Thermo-Calc Documentation Set

Version 2016b

Thermo-Calc Software

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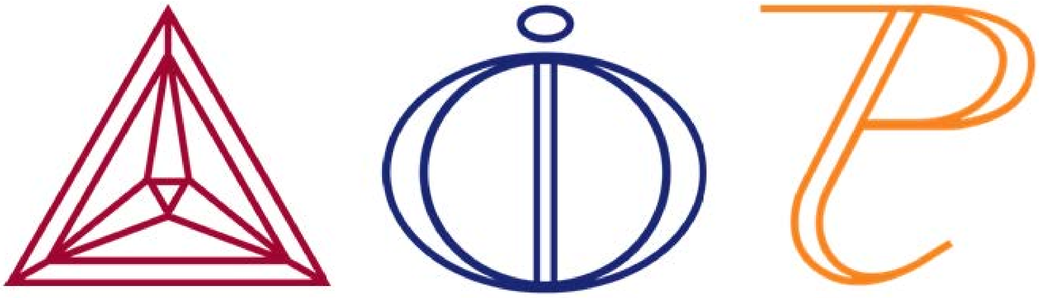
Version 2016b



Thermo-Calc
Software

Windows® Standalone Quick Install Guide

This quick guide helps you do a typical, custom or demo standalone installation. A *standalone* installation is used with the Single-User Node-Locked License (SUNLL), where the software and the license file are together on one computer.

This guide is applicable to:

- Windows operating systems
- Standalone installation (SUNLL) –typical and custom types
- Demo installations – during the installation process you only need to do steps 2 and 3.
- Upgrading to a new standalone version of Thermo-Calc (maintenance plan only)

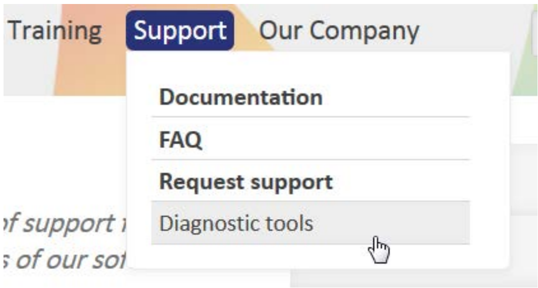
Also see *License and Installation Types* on page 9 for detailed instructions for other operating systems and network installations.

Request a License File

Demo (trial) installations: Skip this section. A license file is automatically installed with the software. You do not need to request it.

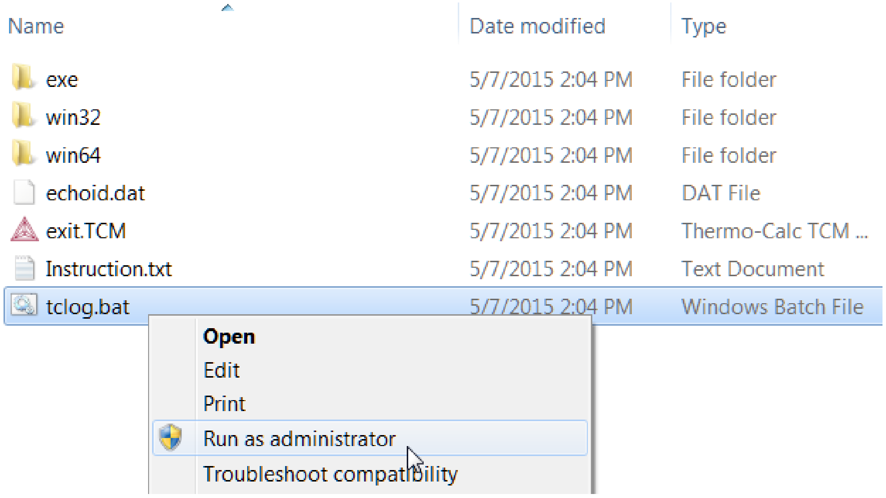
Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

1. Go to Thermo-Calc's website (or click the link sent by email).



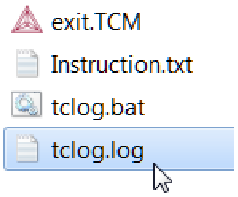
2. Under **TCLOG (Thermo-Calc version S) → Windows computers** click the link **tclog for Windows computers**.

3. Click the **Save file** button and **OK** to download and save the tclog.zip file.
4. Unzip and extract the files.
5. Double-click to open the main folder of the downloaded file. Right-click the **tclog.bat** file and select **Run as administrator**.



Name	Date modified	Type
exe	5/7/2015 2:04 PM	File folder
win32	5/7/2015 2:04 PM	File folder
win64	5/7/2015 2:04 PM	File folder
echoid.dat	5/7/2015 2:04 PM	DAT File
exit.TCM	5/7/2015 2:04 PM	Thermo-Calc TCM ...
Instruction.txt	5/7/2015 2:04 PM	Text Document
tclog.bat	5/7/2015 2:04 PM	Windows Batch File

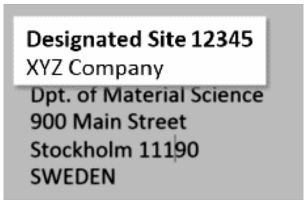
6. Double-click the **tclog.bat** file. Click **Run**. This starts the diagnostic tool and creates a **tclog.log** text file in the same directory.



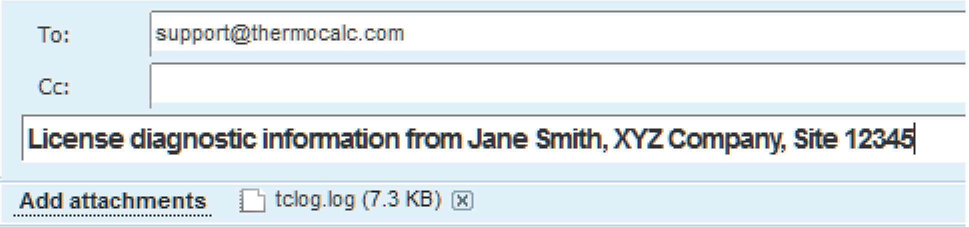
exit.TCM
Instruction.txt
tclog.bat
tclog.log

7. Send an email to support@thermocalc.com and attach the **tclog.log** file. Make sure to include the following in the subject line:

License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*



Designated Site 12345
XYZ Company
Dpt. of Material Science
900 Main Street
Stockholm 11190
SWEDEN


To: support@thermocalc.com

Cc:

License diagnostic information from Jane Smith, XYZ Company, Site 12345

8. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
9. Save the license file(s) to your computer or network.

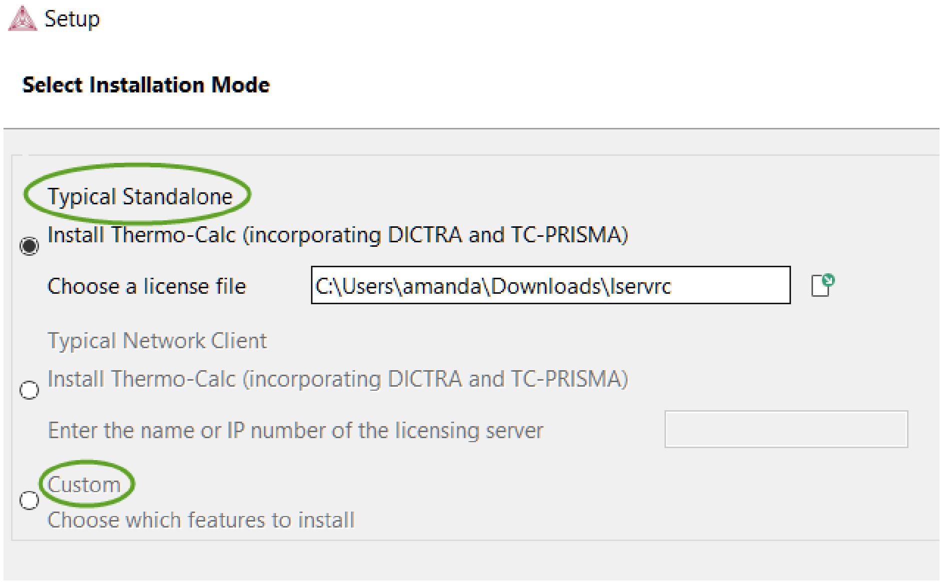
Install the Software

Step 1: Download and run your Thermo-Calc installation software

1. Download the software:
    - *Web downloads*: For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided to download the software.
    - *DVD installations*: Insert the DVD and follow the instructions.
2. Open the Windows folder then right-click the **.exe** file. Choose **Save target as** and save it to your computer. Double-click the **.exe** file to launch the **Setup** program.
3. On the **Setup-Thermo-Calc** window click **Next**.
4. On the **License Agreement window**click to accept the license agreement. Click **Next**.

Demo (trial) installations: Your installation starts and is done when the **Completing the Thermo-Calc Demo Setup Wizard** opens. Click **Finish** and reboot your computer to start using Thermo-Calc.

Step 2: Select the installation mode – typical or custom


Setup

Select Installation Mode

Typical Standalone

● Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)

Choose a license file: C:\Users\amanda\Downloads\lservrc

Typical Network Client

○ Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)

Enter the name or IP number of the licensing server

○ Custom

Choose which features to install

1. In the **Select installation mode** window click **Typical Standalone** or **Custom** to choose specific features to install.

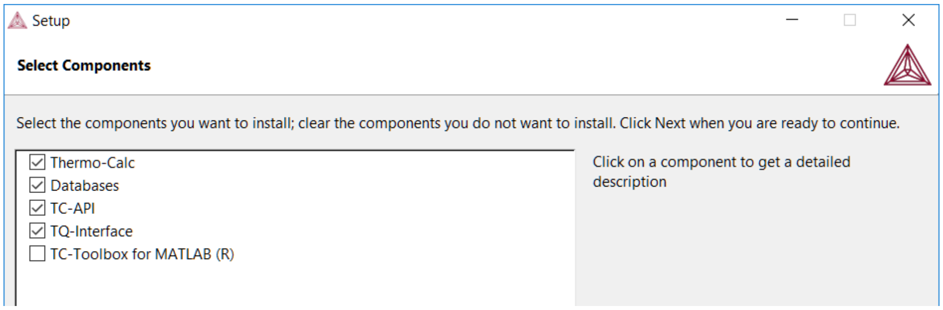
The **Custom** option appears greyed out, but it is available to select.

2. For a **Typical Standalone** installation, in the **Choose a license file** field click the file button to navigate to where you saved the license file emailed to you from Thermo-Calc Software. The license file is called **lservrc**. Click **Next**.

DEMO **Typical Standalone installations**: Your installation starts and is done when the **Completing the Thermo-Calc Demo Setup Wizard** opens. Click **Finish** and reboot your computer to start using Thermo-Calc.

Step 3: Customize your installation

1. In the **Select Components** window, click to select what you want to install. Click **Next**.



Setup

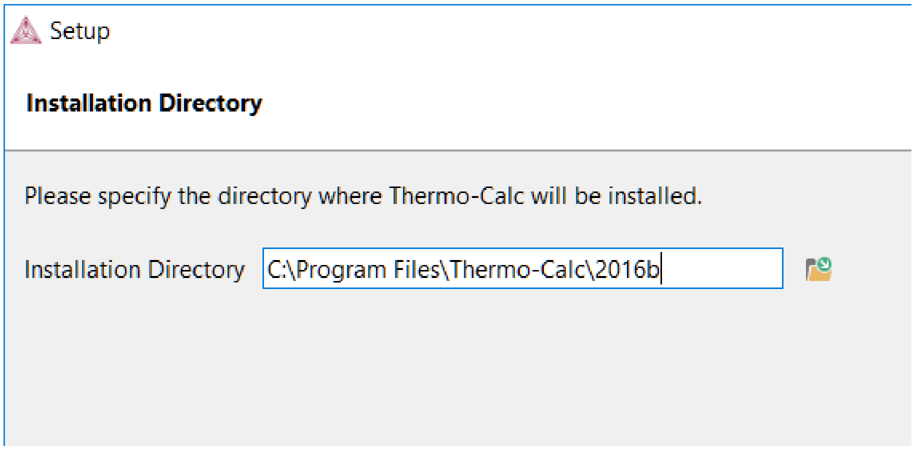
Select Components

Select the components you want to install; clear the components you do not want to install. Click Next when you are ready to continue.

☑ Thermo-Calc
☑ Databases
☑ TC-API
☑ TQ-Interface
☐ TC-Toolbox for MATLAB (R)

Click on a component to get a detailed description

2. In the **Installation Directory** window, either accept the default, enter a file path or click the file button to navigate to another directory.



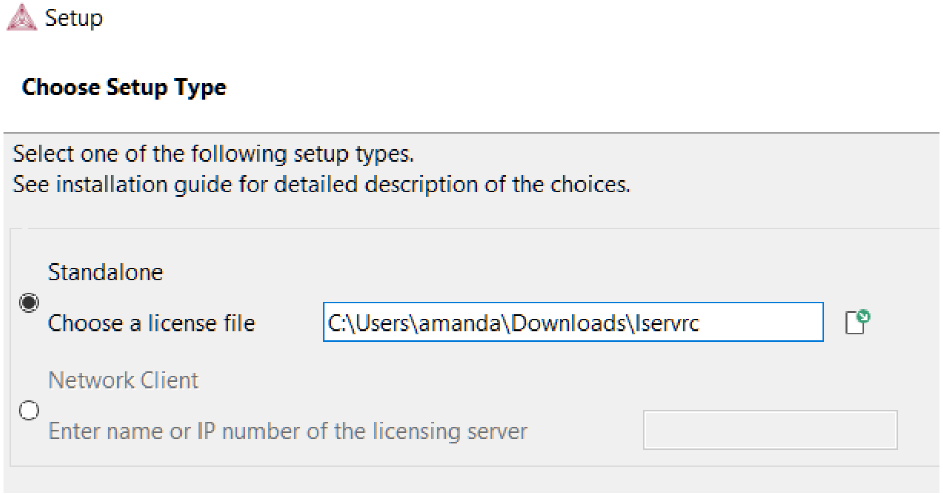
Setup

Installation Directory

Please specify the directory where Thermo-Calc will be installed.

Installation Directory: C:\Program Files\Thermo-Calc\2016b

3. In the **Choose Setup Type** window it defaults to **Standalone**. In the **Choose a license file** field you can accept the default file path or click the file button to navigate to, where you saved the license file emailed to you from Thermo-Calc Software (called **lservrc**). Click **Next**.



Setup

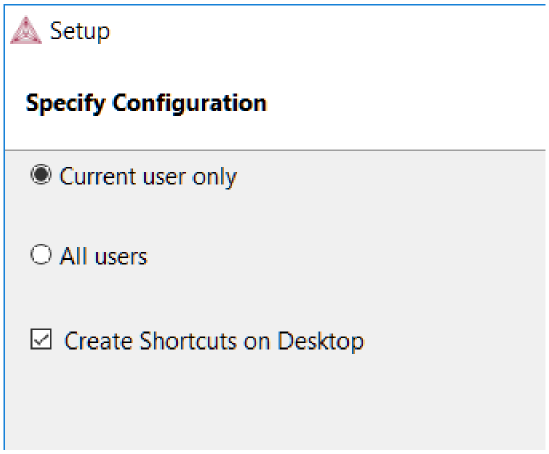
Choose Setup Type

Select one of the following setup types.
See installation guide for detailed description of the choices.

● Standalone
Choose a license file: C:\Users\amanda\Downloads\lservrc

○ Network Client
Enter name or IP number of the licensing server

4. In the **Specify Configuration** window, the default is **Current user only**, meaning the installation is only available for the person logged in and installing the software. Select **All users** to allow anyone using this computer to access Thermo-Calc. By default, the **Create Shortcuts on Desktop** check box is selected. Click **Next**.



Specify Configuration

● Current user only

○ All users

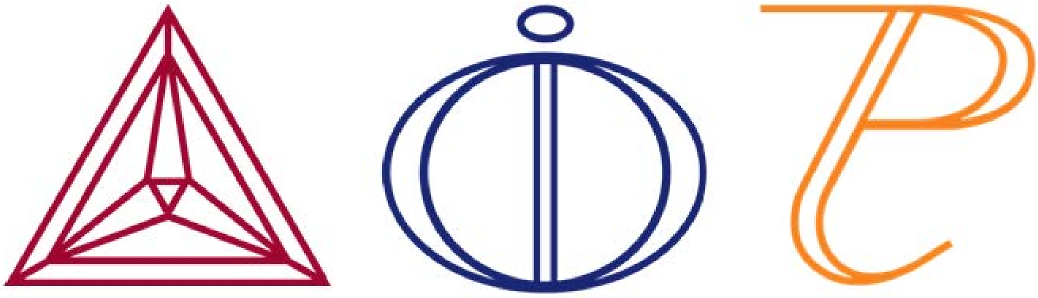
☑ Create Shortcuts on Desktop

5. In the **Ready to Install** window click **Next**. Click **Finish** and start using Thermo-Calc.

Quick Installation Guide: Mac OS®

Standalone Operating Systems

Version 2016b



Thermo-Calc
Software

Mac OS® Standalone Quick Install Guide

This quick guide helps you do a typical or demo standalone installation. A *standalone* installation is used with the Single-User Node-Locked License (SUNLL), where the software and the license file are together on one computer.

This guide is applicable to:

- Mac operating systems
- A typical Standalone installation (SUNLL)
- Demo installations – during the installation process you only need to do steps 1 and 2.
- Upgrading to a new standalone version of Thermo-Calc (maintenance plan only)

Also see *License and Installation Types* on page 9 for detailed instructions for other operating systems and network installations.

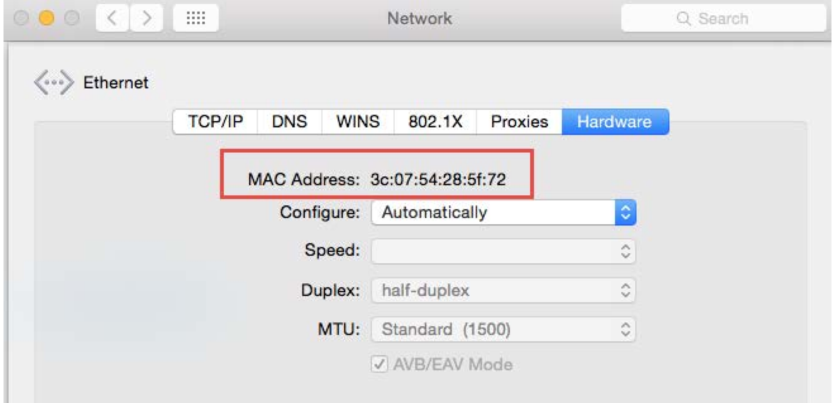
Request a License File

Demo (trial) installations: Skip this section. A license file is automatically installed with the software. You do not need to request it.

Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

1. From the Apple main menu, select **System Preferences**.
2. Click **Network**.

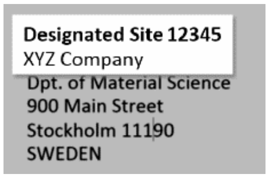
3. In the left column select **Ethernet** or **Built-in Ethernet** (do not select a WiFi connection as a local static MAC address is required).
4. Click **Advanced → Hardware**.
   The **Network** window shows you the **MAC Address**. For example, the MAC address (the host ID) might be **3c:07:54:28:5f:72**.



MAC Address: 3c:07:54:28:5f:72
Configure: Automatically
Speed:
Duplex: half-duplex
MTU: Standard (1500)
☑ AVB/EAV Mode

5. Send an email to support@thermocalc.com and copy and paste the MAC address into the body of the email. Make sure to include the following in the subject line:

License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*



Designated Site 12345
XYZ Company
Dpt. of Material Science
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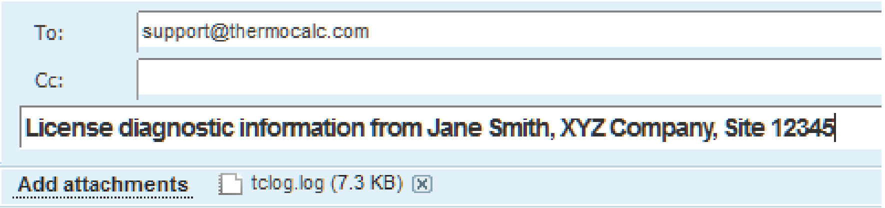
Stockholm 11190
SWEDEN



To: support@thermocalc.com

Cc:

License diagnostic information from Jane Smith, XYZ Company, Site 12345

6. A representative from Thermo-Calc Software replies to the email address provided and attaches your license file or files.
7. Save your license file to your computer or network.

Install the Software

Step 1: Download and install XQuartz

The XQuartz open-source X Windows system is required to run Thermo-Calc on Mac OS X.

1. In a web browser go to https://www.macupdate.com or to download it directly from XQuartz, http://xquartz.macosforge.org/landing/.

2. In the **Search Mac Apps** field, enter *XQuartz*.

3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.7.7.dmg.

4. Click **Download**.

5. Double-click the **XQuartz.pkg** file. Follow the instructions.

6. Click **OK** when the message about logging out displays and click **Close** when the installation is successful.

Step 2: Download and run your Thermo-Calc installation software

1. Download the software:

   - *Web downloads*: For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided to download the software.
   - *DVD installations*: Insert the DVD and follow the instructions.

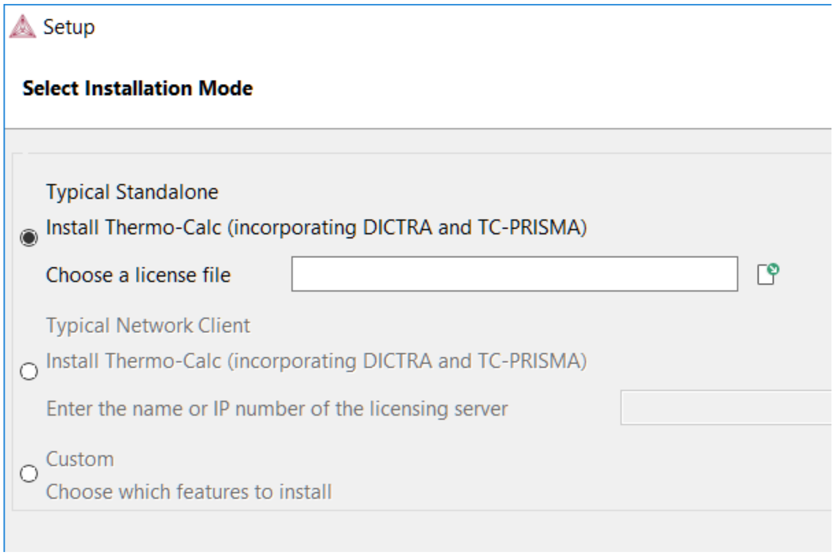
2. Open the Mac folder and right-click the file **Thermo-Calc-2016b-osx.app**. Choose **Download Linked File** and save the installation file to your **Downloads** directory. Unzip the file.

3. On the **Setup-Thermo-Calc** window click **Next**.

4. On the **License Agreement window** click to accept the license agreement. Click **Next**.

Demo (trial) installations: Your installation starts and is done when the **Completing the Thermo-Calc Demo Setup Wizard** opens. Click **Finish** and reboot your computer to start using Thermo-Calc.

Step 3: Select the installation mode



Setup

Select Installation Mode

● Typical Standalone
Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)
Choose a license file

○ Typical Network Client
Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)
Enter the name or IP number of the licensing server

○ Custom
Choose which features to install

1. In the **Select installation mode** window click **Typical Standalone**.

2. In the **Choose a license file** field click the file button to navigate to where you saved the license file emailed to you from Thermo-Calc Software. The license file is called **lservrc**. Click **Next**.

To prevent errors, leave this field blank if you did not get a license file yet.

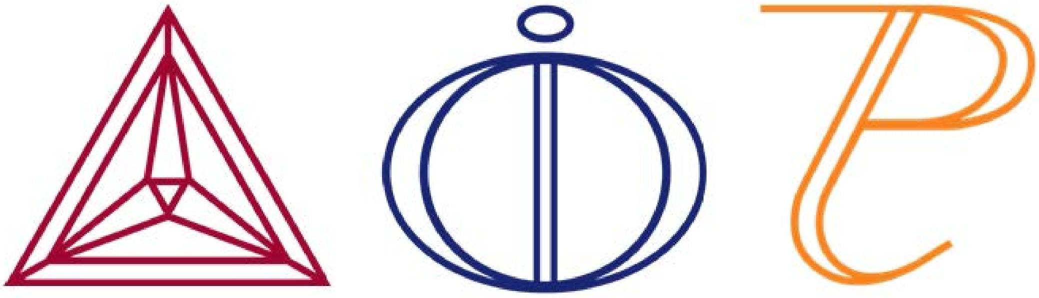
3. The installation starts and is done when the **Completing the Thermo-Calc Setup Wizard** window opens.

4. Click **Finish** and start using Thermo-Calc.

Installation Guide for all Platforms

Windows®, Mac OS® or Linux Operating Systems

Version 2016b



Thermo-Calc
Software

Installing Thermo-Calc

In this section:

System Requirements

A typical installation installs Thermo-Calc and the latest version of the databases.

Additional add-on modules include:

- Diffusion Module (DICTRA)
- Precipitation Module (TC-PRISMA)

You can also install these Software Development Kits (SDKs):

- TQ-Interface (Windows and Linux)
- TC-API (Windows and Linux)
- TC-Toolbox for MATLAB® (Windows only)

System requirements and program availability are available on the web: http://www.thermocalc.com/products-services/software/system-requirements/

Platforms Tested

Thermo-Calc and its components are tested on these platforms:

Windows	**Mac**	**Linux[1, 2]**
Windows 10 64-bit Window 8 64-bit Windows 7 SP1 32-bit Windows 7 SP1 64-bit	Mac OS X El Capitan (10.11.5)	• Ubuntu 16.04 (Xenial) • CentOS 7.0 • OpenSUSE 13.2

[1] Thermo-Calc Software cannot guarantee full functionality if the software is installed on other Linux distributions.

[2] If you are installing on CentOS 7, it is recommended you install gtk2 before you run the installation script.

Key to Using this Guide

This installation guide is for all Thermo-Calc installations running on Windows, Mac OS or Linux operating systems. It is also applicable to demo (trial) installations as well as previously installed versions of Thermo-Calc (the new version is installed alongside the old version).

This guide includes information about:

- The types of licenses and installations available.
- Installing the Thermo-Calc software and its components on stand-alone computers, servers and client computers.
- Installing the license management software for network installations.
- Retrieving and installing license files.
- Troubleshooting to solve common installation problems.

Icons

Name	Description
Information	❗ Provides important information and indicates that more detail is located in the linked or named topic.
Note	✎ The information can be of use to you. It is recommended that you read the text or follow the link to more information.
Operating system	The operating system is indicated when the information is specific to a *Windows*, *Mac OS* or *Linux* operating system.
📁 License file	The license file, which contains the license keys and is installed on either a standalone computer or a network server.
Thermo-Calc	The Thermo-Calc software and its components (including databases) to be installed.

Typographical Conventions

Convention	**Definition**
Forward arrow →	The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, **Tools → Options** is equivalent to: From the **Tools** menu, select **Options**.
Boldface font	A **boldface** font indicates that the given word(s) are shown that way in on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as **Tools → Options**, or to click **Save**.
Italic font	An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
`code` and **`code bold`**	A `code` font indicates you are to make a keyboard entry. It also shows a programming code or code examples. The **`code bold`** font highlights the entry.

Installation Terminology

Term	**Definition**
client computer	A computer without a license file of its own but connected through the network to a computer with the license information. The client computer receives a license token from the computer where the license management software is installed.
consolidated network	A type of network installation where the Thermo-Calc software and a Thermo-Calc licensing software are installed on a single server computer. This allows all computers in the network to access both the software and a license on the server via a client installation.
distributed network	A type of network installation where the Thermo-Calc software is installed on one server computer in a network and the Thermo-Calc licensing software is installed on a different computer. After a thin client installation, all computers in the network can access both the software and the network license key via the server.
host ID	The MAC/Ethernet Address on the computer that a license is locked to.
license file	The file (called *lservrc*) that contains all the purchased license keys. It is issued by Thermo-Calc Software, usually by email.
license key	The information contained in the license file that represents the products purchased and which is then authorised for installation.
License Manager (Windows)	The Windows program used for license management: it distributes license tokens as specified in the network license file issued by Thermo-Calc Software.
License Server (Linux)	The Linux program used for license management: it distributes license tokens as specified in the network license file issued by Thermo-Calc Software.
license server	The use of the term *license server* (lower case letters) is reserved for use for scripts and option files (for example, in an *Unattended Network Client Installations* on page 36). For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the license management program. Also see *License Manager* (Windows) and *License Server* (Linux).
licensing software	The Thermo-Calc license management software. When working in Windows it is called *License Manager* (full name is Sentinel RMS License Manager by SafeNet) and on Linux it is called *License Server* (full name is Sentinel License Sever by Safenet).
Network License (NWL)	The license type used with the licensing software. The NWL can only be used on one specific computer that hosts the licensing software. The Network License uses information about IP addresses and IP ranges to determine which client computers receive license tokens.

Term	Definition
	The software may be used on the number of sites you have paid for and by the number of persons you have paid for on any number of network connected computers
standalone computer	A computer which uses a SUNLL license type.
Single-User-Node Locked-License (SUNLL)	A unique license file for one designated computer at one designated site. It cannot be copied or moved outside the site. If the software is installed on a portable computer, it can be temporarily used off-site. The license can be used without network access (to the License Server).
thin client	An installation where the software is installed on a file server but is run from a client computer. The licensing software may be installed on the file server (consolidated network installation) or on a different computer (distributed network installation).
XQuartz	An open-source X Windows System, which is required to run Thermo-Calc on a Mac.

License and Installation Types

In this section:

License and Installation Types

Installation procedures are based on the license type, the installation type and the operating system.

Demo (trial) installations: Only a standalone installation is available and a license file is automatically installed.

License type	Installation Type	Windows	Mac OS	Linux
SUNLL	Standalone	Yes	Yes	Yes
NWL	Consolidated network	Yes	No	Yes
	Distributed network	Yes	No	Yes
	License installations on a server network	Yes	Yes[1]	Yes

[1] For Mac OS, the licensing software is installed on a Windows or Linux computer server.

www.thermocalc.com/purchase/licensing-options/

About License Keys and Files

Demo (trial) installations: A license file is automatically installed with the software. You do not need to request it.

To run Thermo-Calc and its components you need a valid license key for each product. The license keys are included in the license file emailed to you by Thermo-Calc Software.

You can copy the license file to the applicable computer(s) before or after installing the software—the license file itself is not required during the installation process. However, it is required to make calculations in Thermo-Calc.

Request a License File from Thermo-Calc Software on page 39

Standalone Installations (SUNLL)

The standalone installation is used with the Single-User Node-Locked License (SUNLL). The Thermo-Calc software and a Thermo-Calc license file are installed on a standalone computer. You can do a typical (all operating systems) or a custom installation (Windows and Linux only).

To get started, go to *First Steps of Installation* on page 14 and then *Standalone Installations* on page 20.

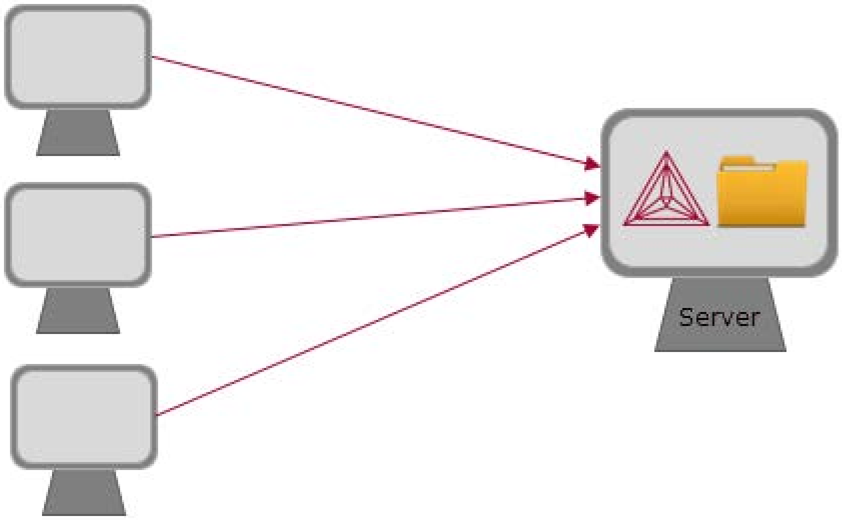
Multi-User Network Installations (NWL)

There are different types of multi-user network installations: consolidated, distributed and where the licensing software is installed on a computer network. There is also a subtype of installation called thin client, which is a step done with the consolidated and distributed network installations.

Thin client installations: A thin client installation is where the Thermo-Calc software is installed on a computer server but is run from a client computer. The licensing software can be installed on the computer server (a consolidated network) or on a different computer (a distributed network). This type of installation is available for Windows and Linux operating systems. The client computer must have the Thermo-Calc software installed. This type of installation mainly sets environmental variables and paths on the client computer.

Consolidated Network Installations

The consolidated network installation is used with a Network License (NWL) and it is available for Windows and Linux operating systems.

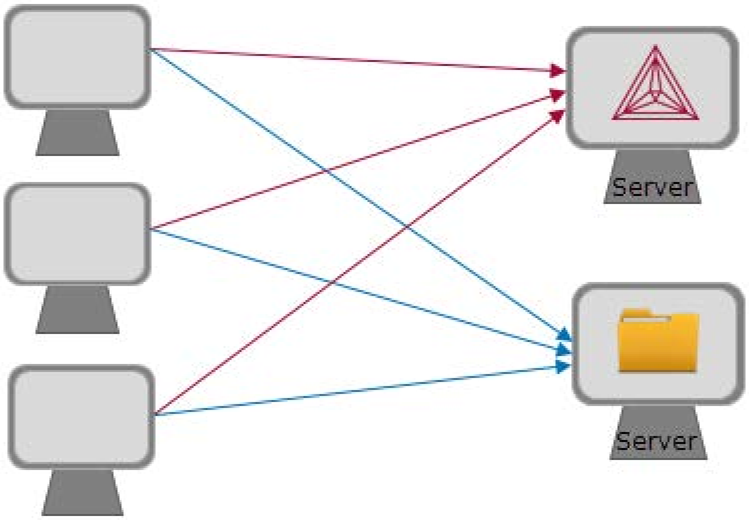


The Thermo-Calc software and the license management program are installed on the same server where the license file 📁 is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the same computer server.

To get started, go to *First Steps of Installation* on page 14 and then *Network Client Installations* on page 26.

Distributed Network Installations

The distributed network installation is used with a Network License (NWL) and is available for Windows and Linux operating systems.

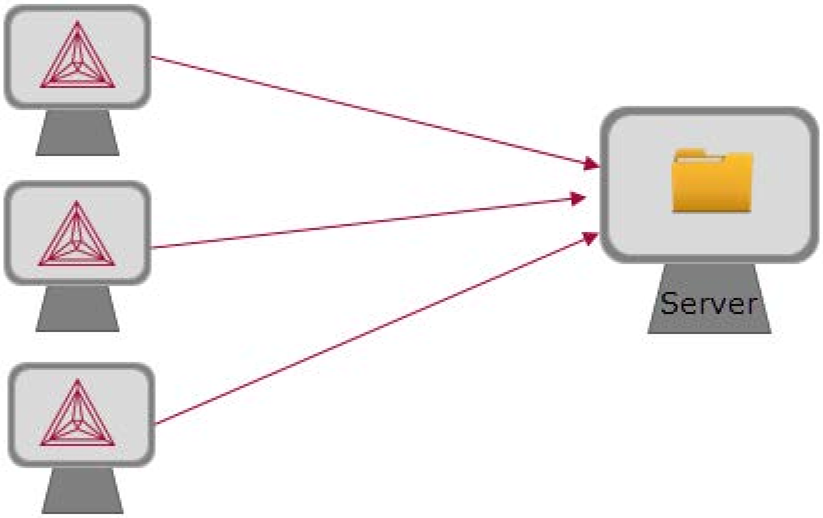


The Thermo-Calc software is installed on one computer server in a network and the licensing software is installed on a different computer server where the license file 📁 is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the two computer servers.

To get started, go to *First Steps of Installation* on page 14 and then *Network Client Installations* on page 26.

License Installations on a Server Network

When a license file is installed on a server network, it is used with a Network License (NWL). It is available for all platforms. However, for Mac OS the server containing the licensing software must be set up on Windows or Linux.



The licensing software is installed on a computer server where the license file 📁 is also copied. The Thermo-Calc software is installed on every computer in the network that needs it.

To get started, go to *First Steps of Installation* on page 14 and then *Network Client Installations* on page 26.

Preparing for Installation

In this section:

First Steps of Installation

This section reviews some of the things you need to do before installing the Thermo-Calc software.

- Learn about the default directories where the software and license files are installed.
- For network installations, collect subnet information.
- For Mac, install XQuartz and make sure the security preferences are set correctly.
- For Linux, install libgfortran 4.4 (or higher).
- For a Linux Cent OS 7 installation, also install gtk2 before you run the installation script.

```
yum install gtk2
```

Should I get my license file before or after software installation? The license file itself is not required during the installation process (and not at all for demo installations). However, it is required to make calculations in Thermo-Calc. The license file has details about your computer(s) that in some cases cannot be determined accurately until *after* installation (especially for a network installation). For most users it is recommended you request the file before you start installing.

Default Directory Locations

The default directories where the software and its components are installed, including where the license file is stored, vary by platform and user type.

On Windows, once Thermo-Calc is installed, you can also locate the Examples and Materials folders, plus all the Manuals using the shortcuts located in the Start menu. Go to **Start →** **All Programs** or **All Apps → Thermo-Calc** and click **Examples**, **Manuals**, or **Materials** as required to open the applicable folder.

If you want to select specific components to install or if you want to install the software in a non-default installation directory, then do a custom installation (Windows and Linux only). In the table, <*user*> stands for the username and <*version*> for the version of Thermo-Calc, for example 2016b.

OS	User type	Default directory
Windows	Normal user	Users\<*user*>\Thermo-Calc\<*version*> Users\<*user*>\Documents\Thermo- Calc\<*version*> **My documents**
	Administrator	Program Files\Thermo-Calc\<*version*> Users\Public\Documents\Thermo- Calc\<*version*>

OS	User type	Default directory
		Public documents
	Custom installation (for all users)	Users\Public\Documents\Thermo-Calc\<*version*>
	License software installations on a server network (the License Manager software)	C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS License Manager\WinNT\
Mac	Administrator (user name and password required)	In the **Applications** folder: Thermo-Calc-<*version*>.app, Thermo-Calc-<*version*>-Demo.app, and, uninstall-Thermo-Calc-<*version*>.app Examples and manuals in /Users/Shared/Thermo-Calc/<*version*> To go to this folder, in Finder, from the **Go** main menu select **Go to folder**. Enter the above file path and click **Go**.
Linux	Non root user	home/<*user*>/Thermo-Calc/<*version*>
	Root user	usr/local/Thermo-Calc/<*version*>
	License software installations on a server network (the License Server software)	If you are doing a network installation then these files are available as a tar-file from the Thermo-Calc Software web site. In the downloaded tar-file, there is a **restart_lserv** script file, which can be used as a template for creating a script that starts up the License Server.

TC-Toolbox for MATLAB

Examples for the TC-Toolbox are placed under MATLAB in the same documents folder as the Thermo-Calc files (My Documents or Public Documents):

`..\Documents\MATLAB\Thermo-Calc-Toolbox-X\Examples`

Where *X* is the installed version number of the toolbox.

For most installations the examples are available in the MATLAB window when the software is opened.

Database Checker Program

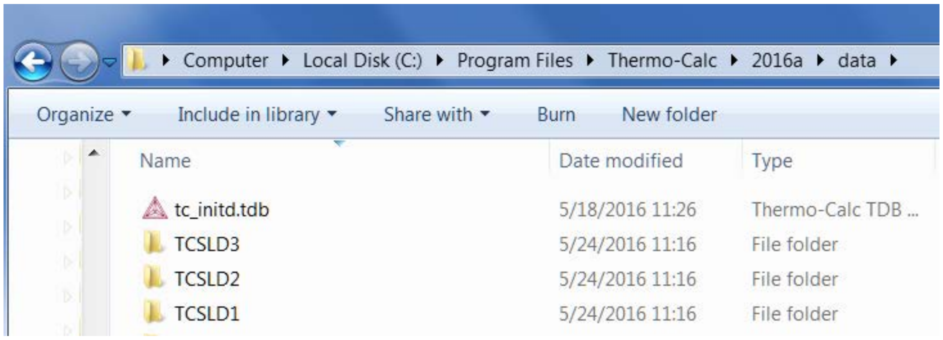
The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.

Thermo-Calc accepts deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and its add-on modules.

The executable **DatabaseChecker** file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu.

Databases

Depending on the type of license and operating system, the encrypted Thermo-Calc databases and the database initialization file are located in a subfolder to the Thermo-Calc installation. For example, in a Windows standalone installation, you can find these in a folder called **data** (file path is *C:\Program Files\Thermo-Calc\<version>\data*).



Name	Date modified	Type
tc_initd.tdb	5/18/2016 11:26	Thermo-Calc TDB ...
TCSLD3	5/24/2016 11:16	File folder
TCSLD2	5/24/2016 11:16	File folder
TCSLD1	5/24/2016 11:16	File folder

Subnet Information for Network Licenses

For network licenses, the subnet information is also required. Contact your company's network administrator for help as required. Additional requirements are included elsewhere for network installations.

- Subnets should be in the format aaa.bbb.ccc*** (for example: 192.168.29.0/24 or 192.168.29.*
- A maximum of six subnets are permitted.
- An alternative way to get this information is to run the command:
- *Windows:* `ipconfig /all`
- *Mac / Linux*: `ifconfig`

Mac OS Installation Notes

Restarting After an Installation

In some types of installations (e.g. a network installation), you may have to restart your Mac to use Thermo-Calc for the first time.

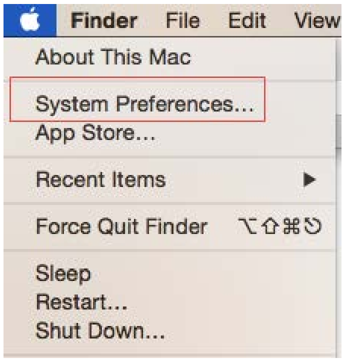
Installing XQuartz

The XQuartz open-source X Windows system is required to run Thermo-Calc on Mac OS X but it is not required to install Thermo-Calc. Before installing Thermo-Calc, you may also need to ensure that the computer security permissions are set.

1. In a web browser go to https://www.macupdate.com or to download it directly from XQuartz, http://xquartz.macosforge.org/landing/.
2. In the **Search Mac Apps** field, enter *XQuartz*.
3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.7.7.dmg.
4. Click **Download**.
5. Double-click the **XQuartz.pkg** file. Follow the instructions.
6. Click **OK** when the message about logging out displays and click **Close** when the installation is successful.

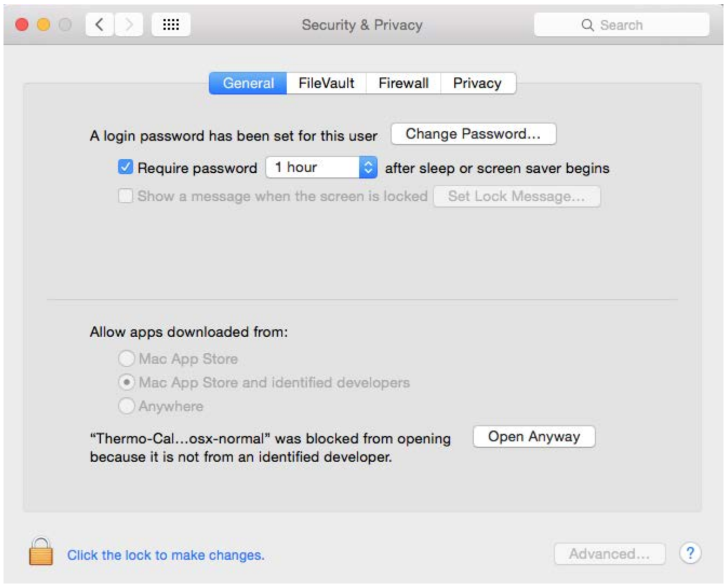
Enabling the Correct Security Settings

1. From the Apple main menu, select **System Preferences**.



2. Click **Security and Privacy**.

3. Click **General**. At the bottom of the **Security & Privacy** window, click the lock icon to make changes. Enter the administrator password as required.



A login password has been set for this user

☑ Require password 1 hour after sleep or screen saver begins

☐ Show a message when the screen is locked

Allow apps downloaded from:

○ Mac App Store
● Mac App Store and identified developers
○ Anywhere

"Thermo-Cal...osx-normal" was blocked from opening because it is not from an identified developer.

Click the lock to make changes.

4. If you have already tried to launch the Thermo-Calc installer, you can click **Open Anyway** to proceed. Otherwise, under **Allow apps downloaded from:** click **Anywhere** and then **Allow from Anywhere**.

5. Continue with the applicable installation type (standalone or network).

Remember to reset your security after installing Thermo-Calc.

Linux Installation Notes

The following are details you need to know regarding your Linux installation as well as how to open Thermo-Calc.

Installing Libgfortran

To install and run Thermo-Calc and its components, a runtime library (libgfortran 4.4 or higher) for GNU Fortran applications is required.

How to install the runtime library

Linux distribution	Notes
openSUSE 13.2	On a standard installation, you do not need to install this runtime library. You may need GCC if it is not already installed on your computer.

Ubuntu 16.04 (Xenial)	Open a terminal and enter the following:
	`> sudo apt-get -y update`
	`> sudo apt-get -y install gfortran`

CentOS 7.0	Open a terminal and enter the following:
	`> sudo yum -y update`
	`> sudo yum -y install libgfortran`

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

Opening Thermo-Calc in Linux

To open Thermo-Calc double-click the **Thermo-Calc-2016b** application or from the Thermo-Calc installation directory enter `$ ./Thermo-Calc-2016b.sh` in the terminal.

Standalone Installations

You can either do a typical or a custom standalone installation. The license type is called a Single-User Node-Locked License (SUNLL).

In this section:

Typical Standalone Installations

The following describes a typical standalone installation. These steps assume you have completed the section *First Steps of Installation* on page 14.

Step 1: Request your license file from Thermo-Calc Software

Demo (trial) installations: Skip this step. A license file is automatically installed with the software. You do not need to request it.

Updates to Thermo-Calc: Customers who subscribe to the annual maintenance plan can skip this step if you have received your license file in an email from Thermo-Calc Software AB. Save the license file to your computer to use during software installation. The license file name must be the same as the existing file name to ensure there are no errors during the update.

Follow the instructions for your operating system in the section *Request a License File from Thermo-Calc Software* on page 39.

Step 2: Download your Thermo-Calc installation software

- *Web downloads*: For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided to download the software.
- *DVD installations*: Insert the DVD and follow the instructions.

Step 3: Run the applicable installation file for your operating system

1. Open the folder for your operating system. Then for:

- *Windows*: Right-click the **.exe** file. Choose **Save target as** and save it to your computer. Double-click the **.exe** file to launch the **Setup** program.
- *Mac*: Right-click the file **Thermo-Calc-2016a-osx.app**. Choose **Download Linked File** and save the installation file to your **Downloads** directory. Unzip the file.
- *Linux*: Right-click the binary file (the BIN file) and save it to your computer. To start the Setup Wizard in a Terminal window, enter these commands in the directory where the binary installation file is saved:

```
> chmod +x linux-installation-x64-2016b.run
> ./linux-installation-x64-2016b.run
```

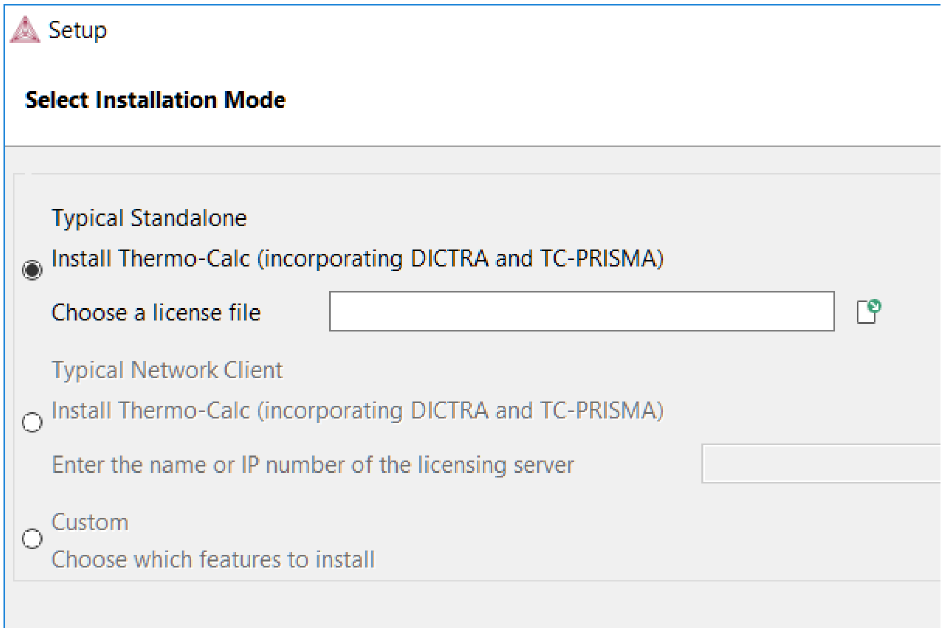
If you are an openSUSE root user, see *Linux Installation Notes* on page 19 for some information about your installation.

2. On the **Setup-Thermo-Calc** window click **Next**.
3. On the **License Agreement window** window click to accept the license agreement.
4. Click **Next**.

Demo (trial) installations: Your installation starts and is done when the **Completing the Thermo-Calc Demo Setup Wizard** opens. Click **Finish** and reboot your computer to start using Thermo-Calc.

Step 4: Select the installation type and upload the license file

1. In the **Select installation mode** window click **Typical Standalone → Install Thermo-Calc (incorporating Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA)**.



Setup

Select Installation Mode

● Typical Standalone
Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)
Choose a license file

○ Typical Network Client
Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)
Enter the name or IP number of the licensing server

○ Custom
Choose which features to install

2. In the **Choose a license file** field enter the path to your license file (called **lservrc**) or click the file button to navigate to a location on the computer (for example, where you saved it). Click **Next**.

To prevent errors, leave this field blank if you did not get a license file yet.

Step 5: Install the software and start using Thermo-Calc

1. In the **Ready to Install** window click **Next**.
2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation and start using Thermo-Calc.

If you did not get your license file see *Request a License File from Thermo-Calc Software* on page 39.

Add New Components to an Existing Installation

If you want to add new components to an existing Thermo-Calc installation (for example, you purchased a license for TC-API), run the executable (Windows) or binary (Linux) installation file again as in Step 3 of *Typical Standalone Installations* on page 21. This is not available for Mac.

1. Double-click the executable Thermo-Calc installation file. Click **Next**.
2. Click to accept the license agreement. Click **Next**.
3. Select the additional component(s) to install. Click **Next**.
4. Click **Next** to start the installation, which adds the new component(s).

Use the **Uninstall** program to *remove* components. See *Uninstalling Thermo-Calc* on page 58.

Custom Standalone Installation

This topic describes how to do a custom installation on a standalone computer for either a Windows or Linux operating system. These steps assume you have completed the section *First Steps of Installation* on page 14.

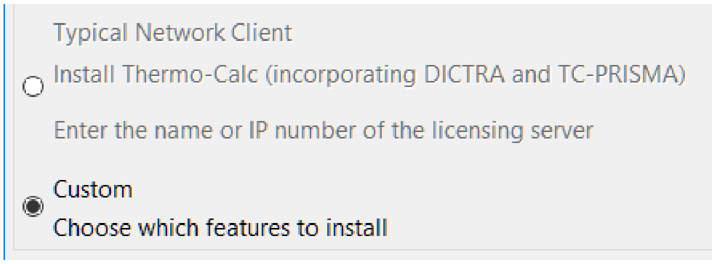
Step 1: Complete Steps 1 to 4 of a typical standalone installation

Follow the instructions for *Typical Standalone Installations* on page 21 to get your license file and to download and run the software.

Step 2: Select the installation type and what components to install

1. On the **Select installation mode** window, click **Custom**. Click **Next**.

The option appears greyed out, but it is available to select.



Typical Network Client

○ Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)

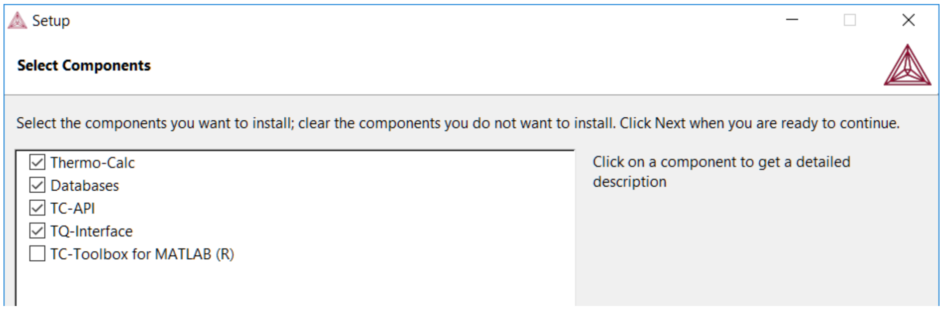
Enter the name or IP number of the licensing server

● Custom

Choose which features to install

2. In the **Select Components** window, click to select what you want to install. Click **Next**.

Additional licenses are required to run TC-API, TQ-Interface, TC-Toolbox for MATLAB (Windows only) and some of the databases. Some elements are included with Precipitation Module (TC-PRISMA) but a separate license is required for full functionality.



Select Components

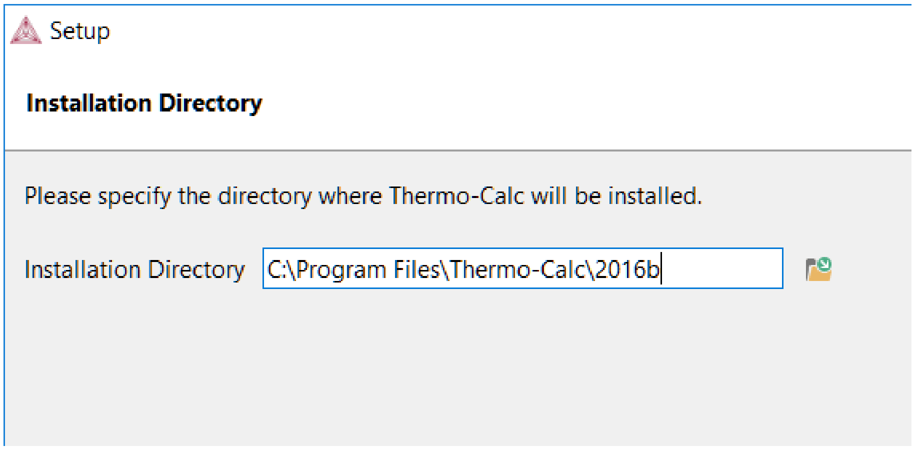
Select the components you want to install; clear the components you do not want to install. Click Next when you are ready to continue.

- ☑ Thermo-Calc
- ☑ Databases
- ☑ TC-API
- ☑ TQ-Interface
- ☐ TC-Toolbox for MATLAB (R)

Click on a component to get a detailed description

Step 3: Set the installation directory path, license file location and shortcuts

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software (see *Default Directory Locations* on page 14). Click the file button 📂 to navigate to another directory. Click **Next**.



Installation Directory

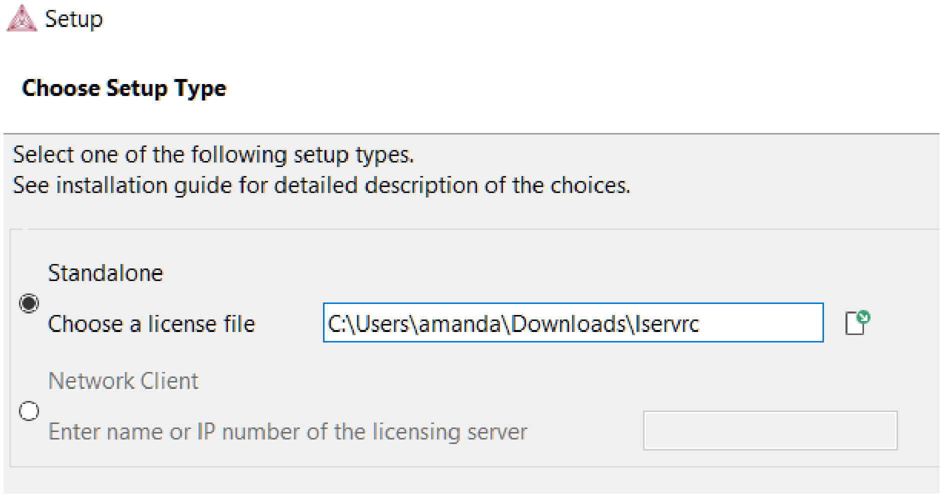
Please specify the directory where Thermo-Calc will be installed.

Installation Directory: C:\Program Files\Thermo-Calc\2016b

For the Windows TC-Toolbox for MATLAB® component, and if you get a **MATLAB not found** message, enter the MATLAB installation directory and click **Next**.

2. In the **Choose Setup Type** window, click **Standalone**.
3. In the **Choose a license file** field enter the path to your license file (called **lservrc**) or click the file button to navigate to a location on the computer. Click **Next**.

To prevent errors, leave this field blank if you do not have a license file yet.



Setup

Choose Setup Type

Select one of the following setup types.
See installation guide for detailed description of the choices.

● Standalone
Choose a license file: C:\Users\amanda\Downloads\lservrc

○ Network Client
Enter name or IP number of the licensing server

4. Set up the Desktop shortcuts.

   For *Windows*, in the **Specify Configuration** window, the default is **Current user only**, meaning the installation is only available for the person logged in and installing the software. Select **All users** to allow anyone using this computer to access Thermo-Calc. By default, the **Create Shortcuts on Desktop** check box is selected. Click **Next**.

   For *Linux*, and if you are installing as a non-root user, by default, the **Create Shortcuts on Desktop** check box is selected. Click **Forward**.

Step 4: Install the software and start using Thermo-Calc

1. In the **Ready to Install** window click **Next** and then click **Finish**.
2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation and start using Thermo-Calc.

If you did not get your license file see *Request a License File from Thermo-Calc Software* on page 39.

Network Client Installations

This installation type is available for Windows and Linux. It is applicable to the consolidated and distributed network types of installations as well as for the licensing installation on a server network.

- Do a *Typical Network Client* installation if you only want to install the Thermo-Calc program (including Diffusion Module (DICTRA)) and Precipitation Module (TC-PRISMA)) and databases.
- Do a *Custom* installation if you want to select specific components to install or if you want to install the software in a non-default installation directory.

In this section:

Typical Network Client Installations

The following outlines how you do a typical network client installation.

Step 1: Install the licensing software

Follow the instructions for your operating system:

- *Set Up the License Manager on Windows* on the next page, or
- *Set Up the License Server on Linux* on page 30

Step 2: Complete Steps 1 to 3 of a typical standalone installation

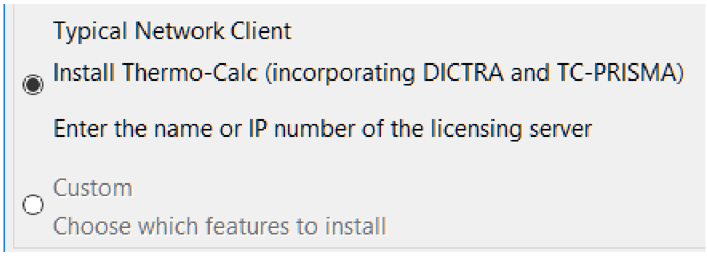
Follow the instructions for *Typical Standalone Installations* on page 21 to download and run the software. It is up to you whether you get the computer information for the license files before or after installing the software.

Step 3: Choose the installation type and enter the computer server details

1. Click **Typical Network Client** installation to install Thermo-Calc incorporating Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA).

The option appears greyed out, but it is available to select.

2. In the field, enter the name or IP number of the computer where the licensing software is installed. Click **Next**.



Typical Network Client

● Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)

Enter the name or IP number of the licensing server

○ Custom

Choose which features to install

Step 4: Install the software and components

1. In the **Ready to Install** window click **Next**.
2. When the **Completing the Thermo-Calc Setup Wizard** window opens, click **Finish**.
3. For *Linux* users, log out and log back in to start using Thermo-Calc.

If you did not get your license file see *Request a License File from Thermo-Calc Software* on page 39.

Set Up the License Manager on Windows

License Manager vs License Server: Both terms refer to the licensing software program installed on a network computer. License Manger is for Windows and License Server is for Linux. See *Installation Terminology* on page 6 for more information.

Installation Requirements

This procedure explains how to install the License Manager on a computer that acts as a license server in your network. It is a Sentinel RMS License Manager Windows service and it supplies the client computers in your network with license tokens when it runs the Thermo-Calc software. A network license can only be used on one specific computer that hosts the License Manager. The network license determines which client computers receive license tokens using their IP addresses and IP ranges.

- For *Mac* installations, the server containing the license file must be set up on a Windows or Linux computer.
- For testing purposes, and in order to confirm the installation is working correctly, install the Thermo-Calc software on the same computer as the Sentinel RMS License Manager. Thermo-Calc can always be uninstalled after testing if required.
- Administrator rights are required.

Installing the License Manager

Step 1: Install the Sentinel RMS License Manager software

1. Follow the instructions to download your Thermo-Calc installation software.
2. Open the directory for Windows and right-click the file **Sentinel RMS License Manager 8.5.1.msi**.
3. Select **Save target as** and choose a suitable directory so that you can easily find the file later.
4. Right-click the downloaded file and choose **Install**. Click **Next**.

Step 2: Choose the installation directory

1. Click to accept the license agreement. Click **Next**.
2. Enter your **User Name** and **Organization** and select to install the License Manager for **All users**. Click **Next**.

3. In the **Destination Folder** window click **Next** to accept the suggested destination directory or **Change** to select another directory. Click **Next**.

Step 3: Choose the setup type and install the software

1. In the **Setup Type** window, select **Complete**. Click **Next**.
2. Select the **Unblock the system firewall for the Sentinel RMS License Manager** check box.

> Selecting the check box is required to runThermo-Calc.

Sentinel RMS License Manager 8.5.1 - InstallShield Wizard

System Firewall Settings Need To Be Modified

The setup program will install the Sentinel RMS License Manager (license server) on this system. To allow communication between the RMS License Manager and the clients running licensed applications, the system firewall settings need to be modified. The Sentinel RMS License Manager will be added to the firewall blocking exceptions list.

Keep the checkbox below selected to unblock the firewall. Clearing this checkbox will let the firewall block the communication between the clients and the RMS License Manager.

☑ Unblock the system firewall for the Sentinel RMS License Manager

Tip: For instructions on unblocking the firewall later, refer to the Sentinel RMS SDK System Administrator's Help.

3. Click **Next** and then **Install**.
4. Click **Finish** to exit the InstallShield Wizard.

Step 4: Copy the license files to the destination directory

Copy the network license file to the destination directory. By default, it is installed in the following directory with the name **lservrc**.

```
C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS
License Manager\WinNT\
```

The name of the **license file** must be in lower case letters (**lservrc**). This is especially important if both Windows and Linux operating systems are part of your network; Linux commands and operations are case-sensitive.

If the default file path does not work, you can set the environmental variable **LSERVOPTS** to select the license file:

a. In the Windows **Control Panel**, go to **System → Advanced system settings**.
b. In **System Properties** select **Advanced → Environment Variables → New**.
c. Enter the **Variable name** LSERVOPTS to specify the parameters with which the License Manager is started.
d. To specify the path to the license file in the **Variable value** field enter the following and include the complete license file path and name.

```
-s <license file path and name>
```

Step 5: Reboot or restart the license manager

Set Up the License Server on Linux

License Manager vs License Server: Both terms refer to the licensing software program installed on a network computer. License Manger is for Windows and License Server is for Linux. See *Installation Terminology* on page 6 for more information.

Installation Requirements

There are a variety of things needed to prepare for a Linux License Server installation. The following points are described in this section.

- You need to stop older versions of the License Server before running the new one. To stop the license server you run **lsrvdown** .
- Root access to your computer is required or you need to be on the **sudoers** list.
- To run the License Server on a Linux 64-bit computer, you need to install 32-bit library support. For example, on CentOS this can be done by running the command:

```
>yum install glib2.i686
```

- You need a valid **lservrc** network license file supplied by Thermo-Calc Software and the actual License Server—a file(program) called **lserv**.

The name of the **license file** must be in lower case letters (**lservrc**) because Linux commands and operations are case-sensitive.

- The license file need to be read and writable by the license server(license manager)
- If you have a license server; Upgrade your license server if the new one is a higher version than the present one. Clients work with newer license servers(managers) but not necessarily with ones older than client.

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

Installing the License Server

Step 1: Stop any older versions of the License Server

Skip this step if this is a new installation.

1. To stop an old version of the License Server that is already running, go to the directory where the old file is found, and enter the commands:

```
>chmod +x <lsrvdown>
>./lsrvdown <host_name>
```

2. Edit existing scripts that start the older version of the License Server so that they start the newer version instead.

For more information about the **lservdown utility**, go to http://sentinelrms.safenet-inc.com/RMSDocumentation/SysAdmin/Content/lsrvdown.htm

Step 2: Write a script to start the License Server

The following is an excerpt from the template script for starting the License Server found in the restart_lserv file.

Replace the paths for LICENSE_SERVER_DIR, LICENSE_FILE_DIR and LOG_DIR to match your system. Save it as a script:

```
# set the directory where the executables are located
LICENSE_SERVER_DIR=/usr/local/Thermo-Calc/2016b/Licensing-files
# set the directory of the license file lservrc
LICENSE_FILE_DIR=/usr/local/Thermo-Calc/2016b/Licensing-files
# set the directory where you wish to save the log-files
LOG_DIR=/tmp
# stop the running server
# (omit this line if calling this script at startup)
$LICENSE_SERVER_DIR/lsrvdown $HOSTNAME
# start the license server
$LICENSE_SERVER_DIR/lserv -s $LICENSE_FILE_DIR/lservrc -l $LOG_DIR/lserv_use.log -f
$LOG_DIR/lserv_err.log
```

Step 3: Confirm the HOSTNAME variable and open the UDP port

1. Before starting the License Server make sure that the value of the $HOSTNAME variable is correct. This value can be shown by typing the `> nslookup $HOSTNAME` command in the terminal window:

   The value should be the same IP address that is shown when you use the ifconfig command.

2. Open the UDP port 5093 in your firewall. In case you have installed SELinux you might also need to disable it by setting `SELINUX=permissive` in the `/etc/selinux/config` file.

Step 4: Start the License Server

1. To start the License Server, run the script created as root. Enter these commands in the console:

   ```
   > chmod +x <name_of_script_file>
   > ./<name_of_script_file>
   ```

2. If you want the License Server to start when you boot the system, put a copy of the start script under `/etc/rc.d/init.d` and start the script from the file `/etc/rc.d/rc.local`.

Thin Client Installations

This topic describes how you install a thin Thermo-Calc client to run Thermo-Calc from a file server. It is applicable to consolidated and distributed network installations for either a Windows or Linux operating system.

Installation Requirements

- You need access to the directory where Thermo-Calc is installed on the file server.
- You need the IP number or name of the computer where the license file is installed.
- For *Linux* you may have to disable your firewall. If SELinux is installed, try disabling it by setting `SELINUX=permissive` in `/etc/selinux/config`.

Installing a Thin Client on Windows

1. Open the **\Thermo-Calc***<version>*\ directory on the file server, where *version* is the current version of the software.
2. Open the directory **Thin-client**. Double-click the `client-install-windows.exe` file.
3. Click to accept the terms of the license agreement. Click **Next**.
4. Enter the name or IP number of where the license file and the License Manager software is installed. Click **Next**.
5. In the **Specify Configuration** window, the default is **Current user only**, meaning the installation is only available for the person logged in and installing the software. Select **All users** to allow anyone using this computer to access Thermo-Calc. By default the **Create Shortcuts on Desktop** check box is selected. Click **Next**.
6. In the **Ready to Install** window, click **Next**.
7. Click **Finish**. To start Thermo-Calc, double-click the desktop shortcut or find the program on the server and start it from there.

Installing a Thin Client on Linux

1. Add the following to the `smb.conf` file, where *<user>* is your user name:

```
[public]

path=/home/<user>/Thermo_Calc/2016b

public=yes

writable=yes

comment=smb share

guest OK=yes

force user=<user>
```

2. From the client, mount the directory on the server computer that contains the Thermo-Calc server installation (by default, this directory is called **/Thermo-Calc/2016b**). How the directory is mounted depends on the Linux distribution being used as well as how the

Thermo-Calc directory on the server computer is shared. Use the Linux command `mount`. For example:

```
> mkdir public
> sudo mount -t cifs //ip_number_server_computer/public ./public -o user=<user>
```

3. Open the mounted directory on your computer, and run `client-install-linux-x64.run` or `client-install-linux-x86.run` in the **/Thin-client** directory.
4. If you do this from the terminal window, use the following to start the installation (assuming that the file server is a 64-bit computer):

```
        > ./client-install-linux-x64.run
```

5. Click **Forward** and click to select the license agreement. Click **Forward**.
6. Enter the name or IP number of the License Server. Click **Forward**.
7. If you are installing as a non-root user, by default, the **Create Shortcuts on Desktop** check box is selected. Click **Forward**.
8. In the **Ready to Install** window click Forward.
9. Click **Finish**. Log out and log back in to start using Thermo-Calc.

Custom Network Client Installations

This section describes how to do a custom network client installation for Windows and Linux operating systems. The requirements are the same as for a typical client installation.

Step 1: Install the licensing software

Follow the instructions for your operating system:

- *Set Up the License Manager on Windows* on page 28, or
- *Set Up the License Server on Linux* on page 30

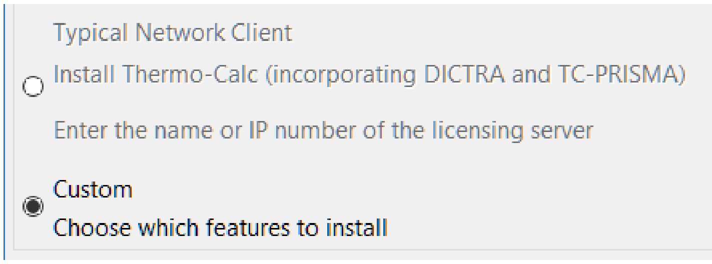
Step 2: Complete Steps 1 to 4 of a typical standalone installation

Follow the instructions for *Typical Standalone Installations* on page 21 to download and run the software. It is up to you whether you get the computer information for the license files before or after installing the software.

Step 3: Choose the installation type and what to install

1. In the **Select installation mode** window click **Custom**. Click **Next**.

The option appears greyed out, but it is available to select.



Typical Network Client

○ Install Thermo-Calc (incorporating DICTRA and TC-PRISMA)

Enter the name or IP number of the licensing server

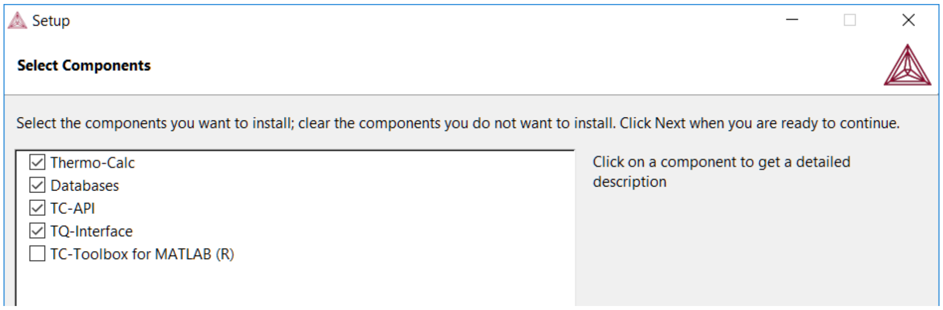
● Custom

Choose which features to install

2. In the **Select Components** window, choose what you want to install. Click **Next**.

Step 4: Set the installation directory path to the license file

1. In the **Installation Directory** window, enter the path to an installation directory (see *Default Directory Locations* on page 14). Click **Next**.



Select Components

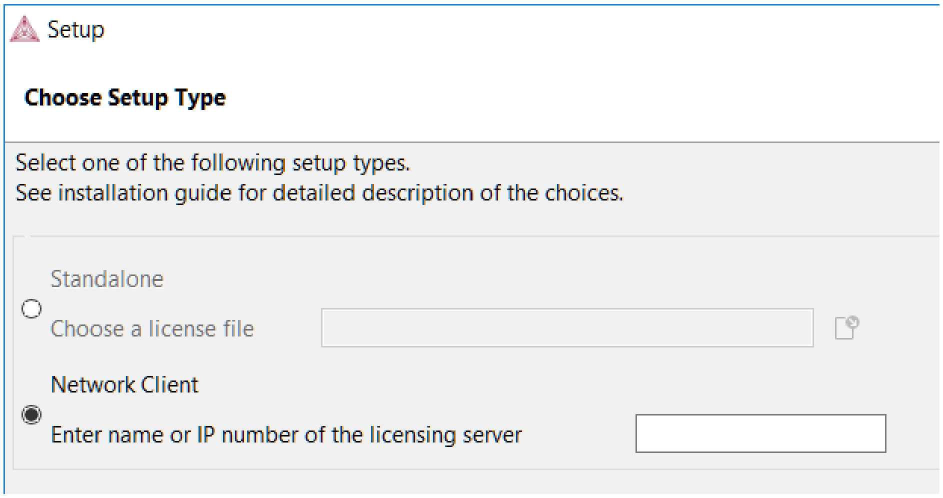
Select the components you want to install; clear the components you do not want to install. Click Next when you are ready to continue.

- ☑ Thermo-Calc
- ☑ Databases
- ☑ TC-API
- ☑ TQ-Interface
- ☐ TC-Toolbox for MATLAB (R)

Click on a component to get a detailed description

For the Windows TC-Toolbox for MATLAB component and if you get a **MATLAB not found** message, enter the MATLAB installation directory and click **Next**.

2. In the **Choose Setup Type** window, click **Network Client** and enter the name or IP number of the computer where the licensing software is installed. Click **Next**.



Choose Setup Type

Select one of the following setup types.
See installation guide for detailed description of the choices.

Standalone

○ Choose a license file

Network Client

● Enter name or IP number of the licensing server

Step 5: Specify the configuration and create shortcuts

For *Windows*, in the **Specify Configuration** window, the default is **Current user only**, meaning the installation is only available for the person logged in and installing the software. Select **All users** to allow anyone using this computer to access Thermo-Calc. By default, the **Create Shortcuts on Desktop** check box is selected. Click **Next**.

For *Linux*, and if you are installing as a non-root user, by default, the **Create Shortcuts on Desktop** check box is selected. Click **Forward**.

Step 6: Install the software and start using Thermo-Calc

1. In the **Ready to Install** window click **Next**.
2. When the **Completing the Thermo-Calc Setup Wizard** window opens, click **Finish**.
3. Log out and log back in and start using Thermo-Calc. If you have not got the license file, go to *Request a License File from Thermo-Calc Software* on page 39.

Unattended Network Client Installations

Terminology note: The use of the term *license server* (lower case letters) is applicable to the option files as described in this section. For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the licensing software.

Sometimes it is convenient to install Thermo-Calc network clients without providing user input after the installation is initiated (an unattended network client installation). This is available for Windows and Linux operating systems.

Make sure you know the name or IP number of the computer where the licensing software and the license file are to be installed.

Step 1: Create an option file in a text editor to enter the options

The following is an example of an option file for a custom network client installation, where *<name/IP number>* is the name or IP number of the computer where the license file is installed and *<MATLAB directory>* is the path to the MATLAB directory (when applicable):

```
installation_mode=custom

setup_type=client

enable-components=thermo,databases,tq,tcapi,toolbox

config=all

icons=1

license_server=<name/IP number>
```

```
matlab_folder=<MATLAB directory>
```

Below is a shorter example, specifying that a typical Thermo-Calc network client should be installed:

```
installation_mode=typical_client
license_server=<name/IP number>
```

Step 2: Go to the directory where the installation file is stored

Thermo-Calc can only be installed in unattended mode from the command line prompt.

Start the installation in unattended mode using the option file created with this command:

- For *Windows*: `<installationfile>.exe – mode unattended --optionfile <path\optionfile>`
- For *Linux*: `<installationfile>.run --mode unattended --optionfile <path/optionfile>`

To see other options when you start the Thermo-Calc installation program from the command line prompt, run this command:

- For *Windows*: `<installationfile>.exe –help`
- For *Linux*: `<installationfile>.run --help`

Request License Files

In this section:

Request a License File from Thermo-Calc Software

The following explains how to retrieve the necessary diagnostic and network adaptor information about your computer and then send an email to Thermo-Calc Software to get your license file(s) containing the license key(s).

To set up the correct licensing (excluding demo installations where a license file is not required):

1. Make a note of your company or organisation's *site number*. You can find the site number on an invoice or any correspondence from Thermo-Calc Software.
2. Retrieve your computer diagnostic and network adapter information.
3. Email Thermo-Calc Software with this information.
4. A Thermo-Calc Software representative emails you the license file. Save the license file **lservrc** (there is no file suffix) to a location where you can easily access it later.

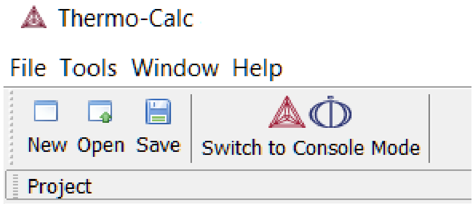
http://www.thermocalc.com/support/request-support/

Getting License Information Using Thermo-Calc

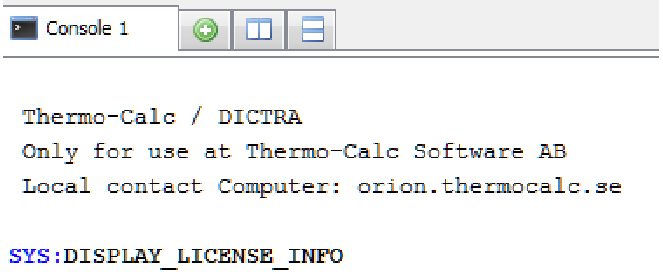
If you have already installed Thermo-Calc, you can view the license information in the GUI. Select **Help → Show License Info**.

In Console Mode you can run the SYS module command DISPLAY_LICENSE_INFO.

1. Open Thermo-Calc.
2. Click **Switch to Console Mode**.

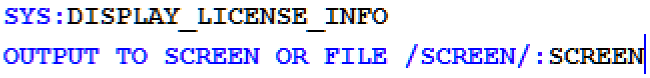


3. At the `SYS:` prompt, enter `DISPLAY_LICENSE_INFO` (all caps).



```
Console 1

Thermo-Calc / DICTRA
Only for use at Thermo-Calc Software AB
Local contact Computer: orion.thermocalc.se

SYS:DISPLAY_LICENSE_INFO
```

4. You can output the information to a `FILE` or to the `SCREEN`.



```
SYS:DISPLAY_LICENSE_INFO
OUTPUT TO SCREEN OR FILE /SCREEN/:SCREEN
```

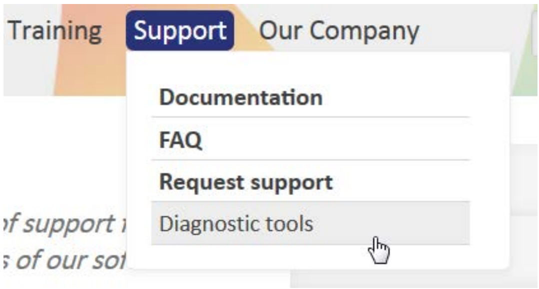
5. For both options, the information is displayed on screen. Copy the section containing the **Ethernet** and **IP address**. You can save it to a text file or paste it directly into an email. If you choose `FILE` as the output, then you can attach the file to an email. For Windows and Linux you can also run the diagnostic program located on the web.

Requesting the License File for Windows

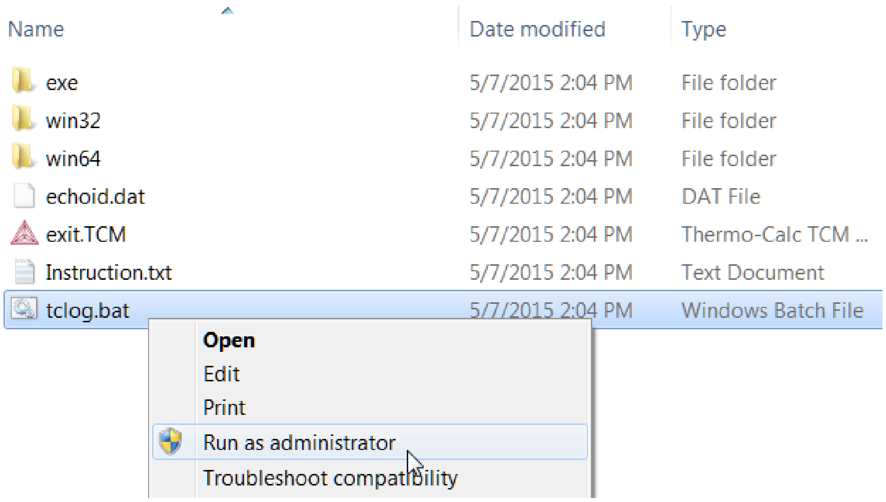
Demo (trial) installations: Skip this section. A license file is automatically installed with the software. You do not need to request it.

Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

1. Go to Thermo-Calc's website (or click the link sent by email).

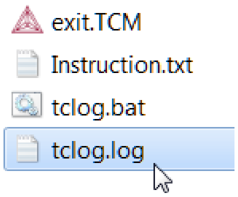


2. Under **TCLOG (Thermo-Calc version S) → Windows computers** click the link **tclog for Windows computers**.
3. Click the **Save file** button and **OK** to download and save the tclog.zip file.
4. Unzip and extract the files.
5. Double-click to open the main folder of the downloaded file. Right-click the **tclog.bat** file and select **Run as administrator**.



Name	Date modified	Type
exe	5/7/2015 2:04 PM	File folder
win32	5/7/2015 2:04 PM	File folder
win64	5/7/2015 2:04 PM	File folder
echoid.dat	5/7/2015 2:04 PM	DAT File
exit.TCM	5/7/2015 2:04 PM	Thermo-Calc TCM ...
Instruction.txt	5/7/2015 2:04 PM	Text Document
tclog.bat	5/7/2015 2:04 PM	Windows Batch File

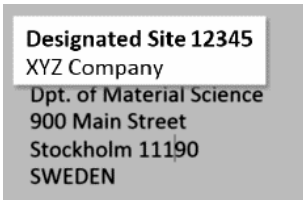
6. Double-click the **tclog.bat** file. Click **Run**. This starts the diagnostic tool and creates a **tclog.log** text file in the same directory.



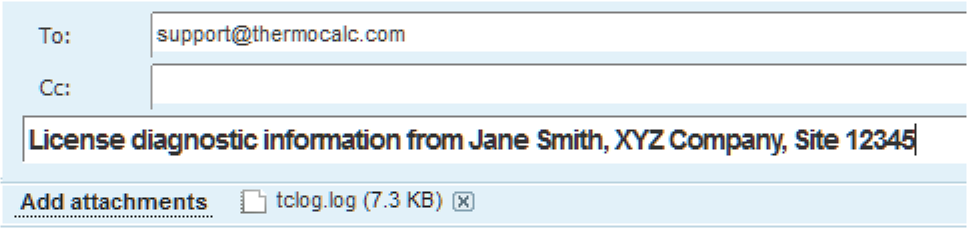
exit.TCM
Instruction.txt
tclog.bat
tclog.log

7. Send an email to support@thermocalc.com and attach the **tclog.log** file. Make sure to include the following in the subject line:

License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*



Designated Site 12345
XYZ Company
Dpt. of Material Science
900 Main Street
Stockholm 11190
SWEDEN



To: support@thermocalc.com

Cc:

License diagnostic information from Jane Smith, XYZ Company, Site 12345

Add attachments tclog.log (7.3 KB)

8. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
9. Save the license file(s) to your computer or network.

Requesting the License File for Mac OS

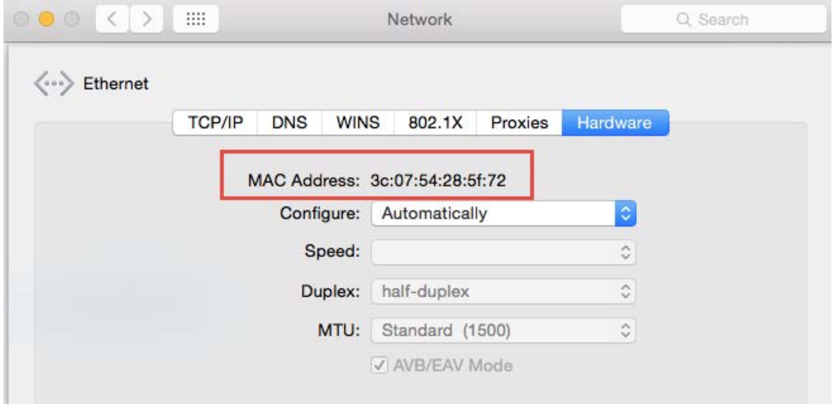
Demo (trial) installations: Skip this section. A license file is automatically installed with the software. You do not need to request it.

Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

1. From the Apple main menu, select **System Preferences**.
2. Click **Network**.

3. In the left column select **Ethernet** or **Built-in Ethernet** (do not select a WiFi connection as a local static MAC address is required).

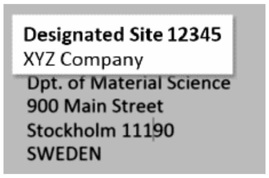
4. Click **Advanced → Hardware**.
   The **Network** window shows you the **MAC Address**. For example, the MAC address (the host ID) might be **3c:07:54:28:5f:72**.



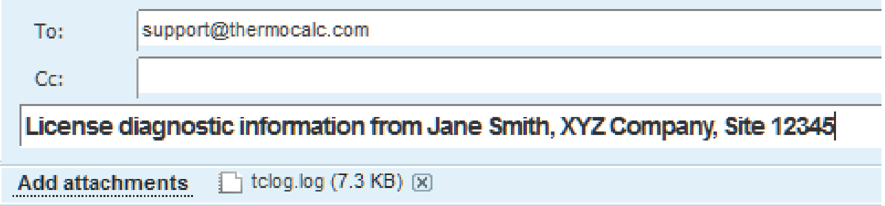
MAC Address: 3c:07:54:28:5f:72
Configure: Automatically
Speed:
Duplex: half-duplex
MTU: Standard (1500)
☑ AVB/EAV Mode

5. Send an email to support@thermocalc.com and copy and paste the MAC address into the body of the email. Make sure to include the following in the subject line:

License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*



Designated Site 12345
XYZ Company
Dpt. of Material Science
900 Main Street
Stockholm 11190
SWEDEN

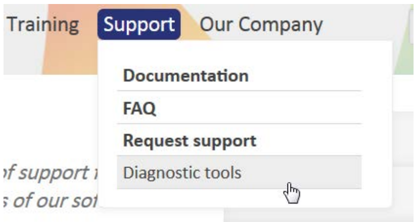


To: support@thermocalc.com
Cc:
License diagnostic information from Jane Smith, XYZ Company, Site 12345

6. A representative from Thermo-Calc Software replies to the email address provided and attaches your license file or files.
7. Save your license file to your computer or network.

Requesting the License File for Linux

1. Go to Thermo-Calc's website.
2. From the **Support** menu select **Diagnostic tools**.



3. Under **TCLOG→ Linux computers** click the link **tclog for Linux computers**.
4. For the **tclog.tar** file, either **Save File** or **Open with** the default program.
5. Go to the **Downloads** directory. Extract the files using the mouse (for example, in Ubuntu right-click to extract the files) or use this command in the Terminal window:

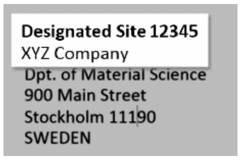
```
> tar -xf tclog.tar
```

6. This creates a subdirectory called *tclog* in the Downloads directory.
7. In a Terminal window run the following command replacing *<tclog_path>* with the path to tclog:

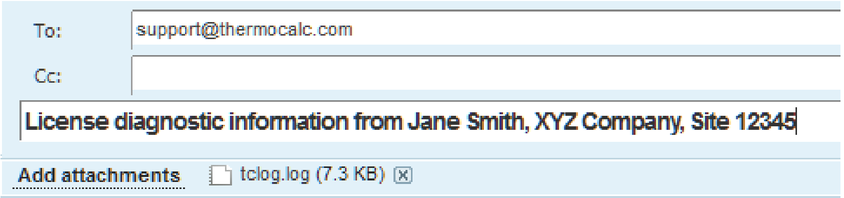
```
> sh /<tclog_path>/script/getreg.sh
```

8. Double-click to open the **tclog** folder. Then either copy the output from the Terminal window or right-click and save the **tclog** file. Name it **tclog.log**.
9. Send an email to support@thermocalc.com and attach the **tclog.log** file. Make sure to include the following in the subject line:

License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*



Designated Site 12345
XYZ Company
Dpt. of Material Science
900 Main Street
Stockholm 11190
SWEDEN



To: support@thermocalc.com
Cc:
License diagnostic information from Jane Smith, XYZ Company, Site 12345

10. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
11. Save the license file(s) to your computer or network.

Troubleshooting

In this section:

License Errors

Issue	**Platform**	**Installation type**	**Action or link to more information**
How do I add or update a standalone (SUNLL) license on a Windows computer where Thermo-Calc is already installed?	Windows	Standalone	*Determining the Current License File Directory Path* on the next page
How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed?	Linux	Standalone	*Determining the Current License File Directory Path* on the next page
How do I add or update a network license on Windows?	Windows	Network	*Determining the Current License File Directory Path* on the next page
How do I add or update a network license on Linux?	Linux	Network	*Determining the Current License File Directory Path* on the next page
No license file found. Copy a valid license file to the installation directory after completing the installation.	All	All	You get this message if the wrong path or no license file is found at a path entered during the installation process. See *Default Directory Locations* on page 14 and *Determining the Current License File Directory Path* on the next page
MATLAB not found (for the TC-Toolbox for MATLAB component)	Windows	All	*MATLAB® Installation Directory* on page 51
Warning Environment variable “LSHOST” is not set. Software will not function properly.	All	Network	*Specifying a New Server Name or IP Number* on page 50
Problem running post-install step. Installation may not complete correctly.	Linux and Mac	Standalone	*Mac OS Installations: Running the License Initialization Script* on page 54 or *Linux Installations: Running the License Initialization Script* on page 55

Issue	Platform	Installation type	Action or link to more information
Unable to run post-installation script, run the license initialization script as root after the installation.			
Firewall warnings related to license management software (License Manager and License Server)	Windows and Linux	Network	*Firewalls* on page 52
Client / Server naming mismatches	Windows and Linux	Network	*Client/Server Mismatch* on page 52
InstallScript engine missing	Windows	Network	You are not notified if the InstallScript scripting engine is not installed. Install the ISScript.msi file and then run the downloaded file from Thermo-Calc again as described in *Set Up the License Manager on Windows* on page 28

Determining the Current License File Directory Path

This topic explains how to find out where your license file is installed, either by default or if a different directory was chosen for previously installed versions. For new installations, where you may not have had a license file when you installed Thermo-Calc (for example, you had a demo version), you can also use these instructions to determine the correct file path.

From Thermo-Calc

If you have already installed Thermo-Calc, you can view the path to the license file in the GUI. Select **Help → Show License Info**.

In Console Mode you can run the SYS module command DISPLAY_LICENSE_INFO.

Windows Standalone Installations

How do I add or update a standalone (SUNLL) license on a Windows computer where Thermo-Calc is already installed?

1. Unpack the .zip file that contains your standalone license and save the LSERVRC file on your computer. Find out where to place the new license file by opening a Command Prompt Window (cmd.exe) and type in the command line:

```
>set LSERVRC
```

2. Press `Enter`. The output from the command is the path to the license file (including the name of the license file). For example: if the output is

```
LSERVRC=C:\Program Files\Thermo-Calc\2016b\lservrc
```

   then the new license file should be placed in `C:\Program Files\Thermo-Calc\2016b\`

Linux Standalone Installations

How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed?

Find out where to place the new license file by opening a Terminal window and type in the command line:

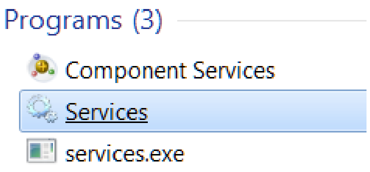
```
echo $LSERVRC
```

Windows Network Installations

How do I add or update a network license on Windows?

1. You need administrator rights to do the following.

- On *Windows 7*, click the Start button and in the search field type Services. Double-click the Services result.



Programs (3)

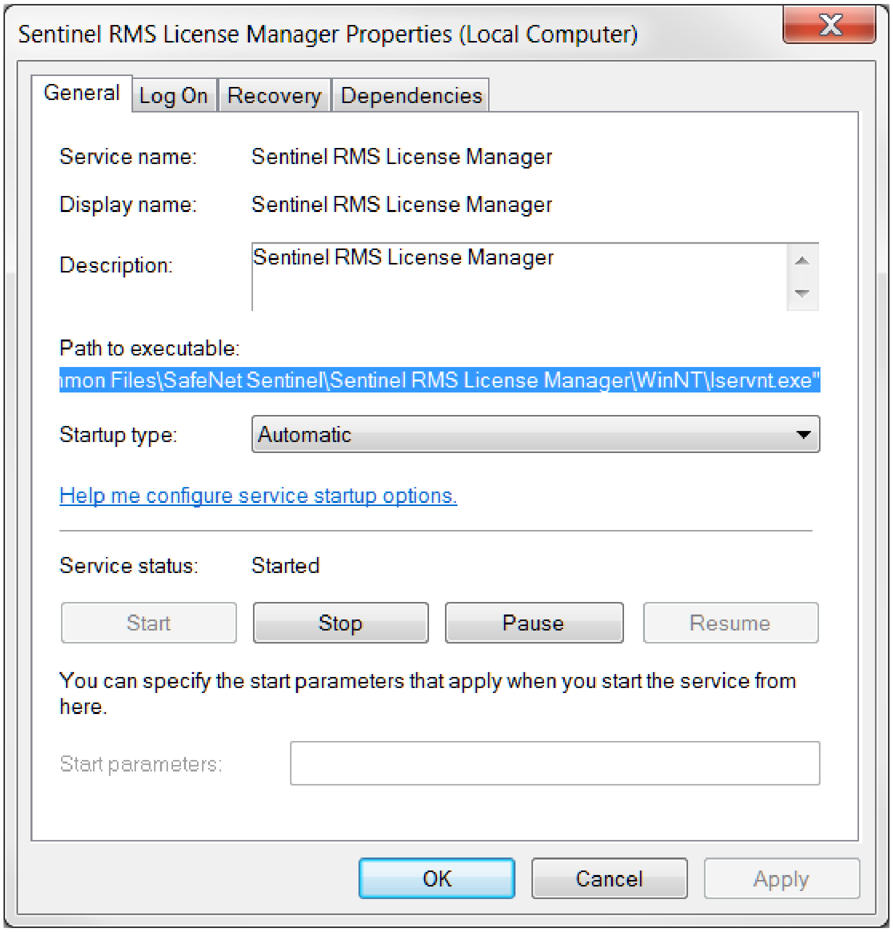
Component Services

Services

services.exe

- On *Windows 8*, move the mouse over the right edge of the screen to access Search, click Settings and then enter and select View Local Services.

2. In the list of installed services, right-click **Sentinel RMS License Manager** and select **Properties** from the pop-up menu.
3. On the **General** tab under **Path to executable**, click the line containing the path to see where the file **lservnt.exe** is located. The license file (lservrc) is in the same directory.



Service name: Sentinel RMS License Manager

Display name: Sentinel RMS License Manager

Description: Sentinel RMS License Manager

Path to executable:
mon Files\SafeNet Sentinel\Sentinel RMS License Manager\WinNT\lservnt.exe"

Startup type: Automatic

Service status: Started

You can specify the start parameters that apply when you start the service from here.

Start parameters:

The default path for the license file is

```
C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS
License Manager\WinNT\LSERVRC
```

4. Move your copy of the license file (lservrc) to this directory.
5. Restart the Sentinel RMS License Manager by:

- Restarting the computer, or
- Right-clicking **Sentinel RMS License Manager** and selecting **Restart** from the list of installed services.

Linux Network Installations

How do I add or update a network license on Linux?

Replace your current license file with the new license file. The license file is located in the same directory as the license server.

Specifying a New Server Name or IP Number

The Thermo-Calc Setup wizard does not warn you if the name or IP number entered to the server (with the license management software) is incorrect.

If the name or IP number is not set at all, or if it is set to an empty string, then when you start Thermo-Calc the following message displays: *Warning Environment variable "LSHOST" is not set. Software will not function properly*.

Windows

Changing the server name or address (Windows)

This section explains how to specify or change the name or IP number of the server where the License Manager is installed and for a consolidated network client installation.

To install a license for an existing Thermo-Calc program, follow these steps:

1. Close all running Thermo-Calc programs.
2. Open a command line window.

- In *Windows 8*, use Search (mouse-over the right edge of your screen) to find **cmd** and then double-click the Command line icon.
- In *Windows 7*, from the Start menu click **Run** and type **cmd** in the field.

3. Specify the name or IP number of the licensing software server. Type:

```
set LSHOST=<name/IP number>
```

To display the current name or IP number, type:

```
set LSHOST
```

Mac

Mac installations

Permanently set the environmental variable LSHOST to specify a new licensing server name or IP number. Refer to the file /Applications/Thermo-Calc-2016b.app/Contents/plist.info.

In this file, you can manually set the TC61_HOME variable, which specifies the home directory of the Thermo-Calc program. See the plist.info file for an example.

Linux

Linux installations

You can set or change the name or IP number of the license server at a later time by setting the environmental variable “LSHOST” to this name or number.

MATLAB® Installation Directory

For Windows installations of the TC-Toolbox for MATLAB component, you may get an error message or window asking for the MATLAB installation directory path. If it is during the installation Setup process, enter the path in the field.

Determining the licensing software version

Sometimes you may need to know the version of License Manager (Windows) or License Server (Linux) software being used. This can be useful while troubleshooting network installations.

- On *Windows* open a command prompt and go to the directory where `lservnt.exe` is found. For example:

  ```
  >C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS
  License Manager\WinNT
  ```

  Type the command `>lservnt.exe -help` and the version is displayed.

- On *Linux* open a Terminal window and go to the directory where the `lserv script` is saved. For example:

  ```
  >cd /usr/local/Thermo-Calc/<version>/Licensing-files
  ```

  Type the command `>./lserv -help` and the version is displayed.

Firewalls

Windows

For a Windows License Manager installation you may have to change the system firewall settings to allow the License Manager to communicate with the computers running the client applications. Go to the Windows Firewall settings window to see if there are any problems. If prompted, select Unblock the system firewall for the Sentinel RMS License Manager and click Next.

Linux

For a Linux License Server installation you need to open the UDP port 5093 in your firewall. In case you have installed SELinux you might also need to disable it by setting SELINUX=permissive in the /etc/selinux/config file.

Client/Server Mismatch

For some network installations there can be a naming mismatch that causes errors. The server (where the license management software is installed) gets information from its DNS servers that an IP address (aaa.bbb.ccc) belongs to a computer (Computer A). But the client computer identifies itself as having a different IP address (aaa.bbb.ccc.eee) for the same computer (Computer A).

Even if the IP address of the client computer belongs to a subnet range listed in the license file, there is a problem with accessing the license file because the computer name does not match the information.

You may need your organisation’s network administrator to assist with this issue.

How to Check

Step 1: Compare computer names on the client computer and server

1. On the client computer, start a command prompt **cmd.exe** and type `ipconfig /all`.

Press `Enter`. A variety of data is displayed on screen. Write down the following information for later comparison:

- Host name
- Dns Suffix
- Current IPv4 Address

2. In the command window, type `nslookup` *<client_computer_name>,* where *client_computer_name* is the actual name of the client. Press `Enter`.

   This shows what information is saved on the DNS Servers used by the client computer. This information should match what is shown in the output from the first step.

3. On the server that holds the license management software, open a command prompt and run the command line: `nslookup client_computer_name`. The output lists the information for this server.

   Does it match the information given by the command ipconfig /all on the client computer? If not try the following:

Step 2: Try these options to correct the issue

1. If the client computer has a dynamic (DHCP) IP address, either change it to a static one or make a reservation on the DHCP Server so that the computer always get the same IP address.
2. Update the records on the DNS Servers used by both the client computer and the server computer.

You can also hard code computer names and IP addresses in the local "address book" of the client and server:

1. On the client computer, make a backup copy of the file C:\Windows\System32\drivers\etc\hosts.
2. Open the original in a simple text editor.
3. Add a new line which contains the IP and name of the server, for example: 192.168.29.27 license_server.thermocalc.se.
4. Save the changes.
5. On the server, make a backup copy of the file /etc/hosts.
6. Open the original in a simple text editor.

7. Add a new line which contains the IP and name of the client, for example: 192.168.29.47 Computer_A.thermocalc.se.
8. Save the changes.
9. In the host file, there is an example of how the operating system (Windows or Linux) wants the line in the hosts file to look like.

Mac OS Installations: Running the License Initialization Script

As part of the Standalone installation of Thermo-Calc, the Setup runs a license initialization script. If this part of the installation process did not complete properly for a standalone installation, you must manually run the license initialization script. You need the administrator username and password for these steps.

How to Run the Script

For this script to successfully initialize the license, the license file must be called lservrc and be located in the folder /Applications/Thermo-Calc-2016b.app/Contents/Resources or /Applications/Thermo-Calc-2016b-Demo.app/Contents/Resources for demo installations.

Also see *Default Directory Locations* on page 14.

1. Open a terminal window. The **Terminal** application is in the */Applications/Utilities* folder.
2. At the prompt, enter this command:

```
$ sudo /Applications/Thermo-Calc-
2016b.app/Contents/Resources/license-initialization-MacOS-x86_64.sh
```

   For demo installations, the path should be `/Applications/Thermo-Calc-2016b-Demo.app/Contents/Resources/ license-initialization-MacOS-x86_64.sh`.

   If you are not already logged in as an administrator, you probably cannot run the `sudo` command. If this is the case, then you can use the `su` command in the terminal window to login as an administrator. Contact your local system administrator for help.

3. Enter the administrator password and press `Enter`.
4. When you restart your computer and run the license initialization script, you are ready to start using Thermo-Calc.

If you did not install a license file during this procedure, you can still start Thermo-Calc although you will get the **No license file found** message.

Linux Installations: Running the License Initialization Script

As part of a Standalone installation of Thermo-Calc, the Setup runs a license initialization script. If you get a warning message during the standalone installation Unable to run post-installation script, run the license initialization script as root after the installation, then you need to manually run the script as root.

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

How to Run the Script

For this script to successfully initialize the license, the license file must be called **lservrc** and be located in the directory where you have installed Thermo-Calc.

Also see *Default Directory Locations* on page 14.

1. In the console, go to the Thermo-Calc installation directory.

   The default installation directory is `/home/<user>/Thermo-Calc/2016b` if you are installing as a non-root user, where <user> is your user name. If you are installing as root, then this directory is `/usr/local/Thermo-Calc/2016b`.

2. Enter this command:

   ```
   $ sudo sh license-initialization-linux-x86_64.sh
   ```

   If you are not able to execute the `sudo` command because you are not on the sudoers list, you must log in as a root user with the command `su`, and then use `sh` to run the license initialization script. For example, on a 64-bit computer, enter the following:

   ```
   $ sh license-initialization-linux-x86_64.sh
   ```

3. Log out of Thermo-Calc and then log back in to save these changes.

Uninstalling Thermo-Calc

In this section:

Uninstalling Thermo-Calc

Windows 10

1. From the **Control Panel** Desktop app, go to **Programs → Programs and Features → Uninstall or change a program**.
2. In the list of programs, locate the version of Thermo-Calc you want to uninstall. Click to highlight that row.
3. Click **Uninstall/Change**.
4. In the **Setup** window, **Uninstallation Mode** dialog box, choose to uninstall the **Entire application** or **Individual components**. Follow the instructions to finish.

Windows 7

1. From the **Start** menu, go to **All Programs** or **All Apps → Thermo-Calc**.
2. Click **Uninstall-Thermo-Calc***<version>*.
3. In the **Uninstallation Mode** window, choose to uninstall the **Entire application** or **Individual components**. Follow the instructions to finish.

Mac

Deleting the program from the Applications folder does not remove the program from your operating system. Run the **Uninstall-Thermo-Calc***<version>* program located in the Applications folder. This is also applicable to the Demo version of the software.

1. Go to the **Applications** folder and double click the file that starts with **Uninstall-Thermo-Calc***<version>*. Enter the administrator's user name and password.
2. Click **Yes** in answer to the question **Do you want to uninstall Thermo-Calc and all of its modules?** Click **No** to quit.
3. The **Uninstalling Thermo-Calc** window shows the progress. Click **OK** when prompted.

Linux

1. To start the uninstallation procedure, in the Thermo-Calc installation directory use the command
   ```
   ./uninstall-Thermo-Calc-2016b
   ```
   For *Thin Client* installations, use the command `/uninstall-Thermo-Calc-Client-2016b`
2. To remove the whole application, including all its components, select **Entire application** and click **Forward**, or to remove specific components, select **Individual components**

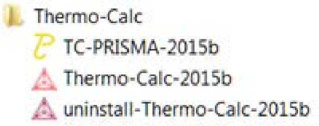
and click **Forward**.

If you intend to reinstall Thermo-Calc 2016b it is important to remove the environmental variable TC61_HOME by logging out and back into the Linux user account.

Uninstalling Standalone Versions of TC-PRISMA

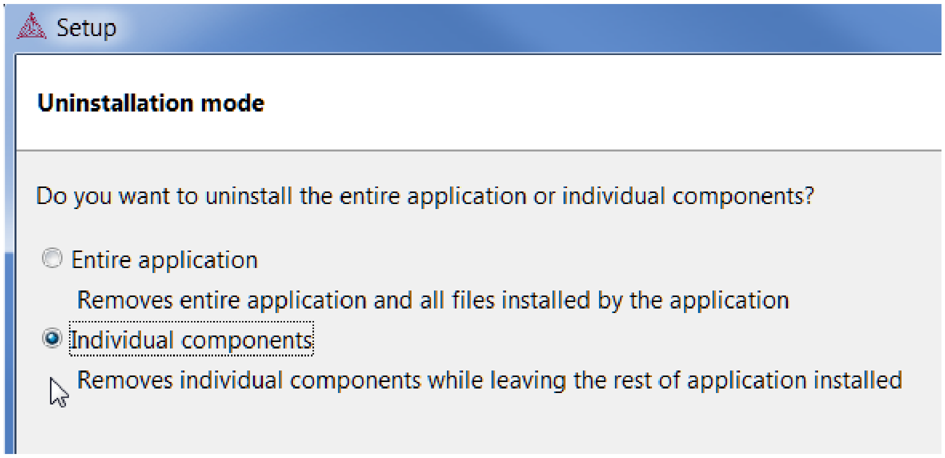
As of Thermo-Calc version 2016a, TC-PRISMA is no longer a standalone program. It is integrated into the Thermo-Calc Graphical Mode and considered an add-on module called the Precipitation Module. It is also available for all platforms (Windows, Mac and Linux). If you have older versions of the TC-PRISMA software that you want to uninstall, follow these instructions.

1. Go to the Thermo-Calc uninstaller. For example, in Windows 7, go to **Start → All Programs → Thermo-Calc** or in Windows 10 go to **Start → All Apps → Thermo-Calc**.
2. Click **uninstall-Thermo-Calc-2015b** (or the version of TC-PRISMA you have).



Thermo-Calc
TC-PRISMA-2015b
Thermo-Calc-2015b
uninstall-Thermo-Calc-2015b

3. In the **Setup** window, click **Individual components**. Click **Next**.



Setup

Uninstallation mode

Do you want to uninstall the entire application or individual components?

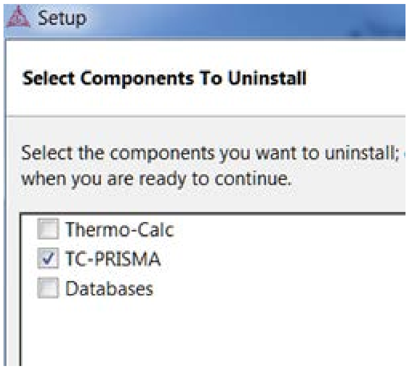
○ Entire application

Removes entire application and all files installed by the application

● Individual components

Removes individual components while leaving the rest of application installed

4. Select the **TC-PRISMA** check box.



Setup

Select Components To Uninstall

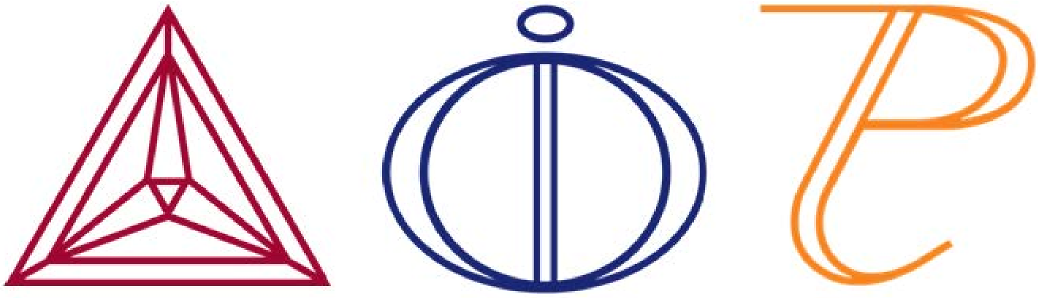
Select the components you want to uninstall;
when you are ready to continue.

☐ Thermo-Calc
☑ TC-PRISMA
☐ Databases

5. Click **Next** and then **OK** when the software component is uninstalled.

Thermo-Calc User Guide

Version 2016b



Thermo-Calc
Software

Introduction to Thermo-Calc

This guide is an introduction to working with both *Graphical Mode* and *Console Mode* in Thermo-Calc.

In this section:

The Thermo-Calc Software

The Thermo-Calc software is a sophisticated database and programming interface package used to perform thermodynamic calculations. It can calculate complex homogeneous and heterogeneous phase equilibria, and then plot the results as property diagrams and phase diagrams.

The Thermo-Calc software (also referred to as the *Thermo-Calc program* or *the software* to distinguish it from the company name) fully supports stoichiometric and non-ideal solution models and databases. These models and databases can be used to make calculations on a large variety of materials such as steels, alloys, slags, salts, ceramics, solders, polymers, subcritical aqueous solutions, supercritical electrolyte solutions, non-ideal gases and hydrothermal fluids or organic substances. The calculations take into account a wide range of temperature, pressure and compositions conditions.

A Software Development Kit (SDK) is available. This SDK is used to plug the calculation engine into your own application or into other third-party applications.

The Thermo-Calc program also includes modules to run simulations of:

- Diffusion controlled transformations in multicomponent systems: Diffusion Module (DICTRA)and DIC_PARROT.
- Diffusion controlled multi-particle precipitation process in multicomponent and multi-phase alloy systems: Precipitation Module (TC-PRISMA).

All Thermo-Calc users have access to the Precipitation Calculator to use it with two elements. To fully realise the power of the Precipitation Module you need an additional license key. There are also two examples available to all users. All examples use demonstration databases, which are included with every installation.

Use online help for information about how to use Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA).

Typographical Conventions

The following typographical conventions are used throughout the documentation:

Convention	Definition
Forward arrow symbol →	The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, **Tools → Options** is equivalent to: From the **Tools** menu, select **Options**.
Boldface font	A **boldface** font indicates that the given word(s) are shown that way on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as **Tools→Options**, or to click **Save**.

Convention	**Definition**
Italic font	An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
COMMAND	For features in Thermo-Calc that use the command line, this font and all capital letters indicates that this is a COMMAND used in the Console Mode terminal. Examples of how you can use a command are written with code font: Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE and choose `Elements`).
HELP	Text in blue and underline and a page number is a link to another topic in the current or referenced guide. Often command names are also topics. Clicking the link takes you to more detail about a particular command or subject in the PDF.
<Enter>	Text with <angle brackets> indicates a keyboard entry. Usually to press <Enter> (or Return).
`code` and **`code bold`**	A `code` font shows a programming code or code example. The **`code bold`** font highlights the entry.
Important	Provides important information and indicates that more detail is located in the linked or named topic.
Note	The information can be of use to you. It is recommended that you read the text or follow the link to more information.
Also see	Go to more information about the topic being discussed.
Examples	Go to the example collection to learn more.

Graphical Mode vs Console Mode

There are two interfaces in Thermo-Calc: *Graphical Mode* with a graphical user interface (GUI) and *Console Mode*, which uses a command line interface.

- In Graphical Mode calculations are set up, carried out, and visualized as part of a *project*. The steps in the project are performed with *activities*. There are templates and a

Wizard available to guide you through the process of defining the project.

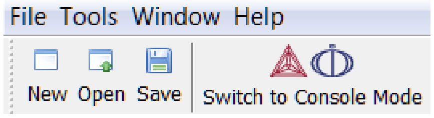
- In Console Mode you work with *modules*, which are managed using commands typed at a prompt. Some modules, called *response-driven modules*, prompt you with a series of questions that typically take you through the process of defining your system, setting calculation conditions, performing calculations and plotting the results.

Switching Between Modes

The first time you open Thermo-Calc, it defaults to Graphical Mode. For any future instance it defaults to the last mode used.

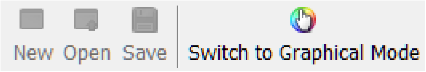
Along the top of the GUI is the toolbar where you switch between modes.

The toolbar in Graphical Mode



The toolbar in Console Mode

In Console Mode, except for the **Switch to Graphical Mode** button, the toolbar is not used.



See *Main Menu and Toolbar* on page 33 for information about the **Tools**, **Window** and **Help** menus, which are available in both modes.

The two modes can be run simultaneously, but there is no communication between them. What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. One exception is the plot settings. See *Global Settings: Graphical and Console Mode-Plotting* on page 202.

Although many calculations can be done in either mode, only data optimization and thermodynamic or kinetic assessments are available in Console Mode.

Help Resources

Online and Context Help

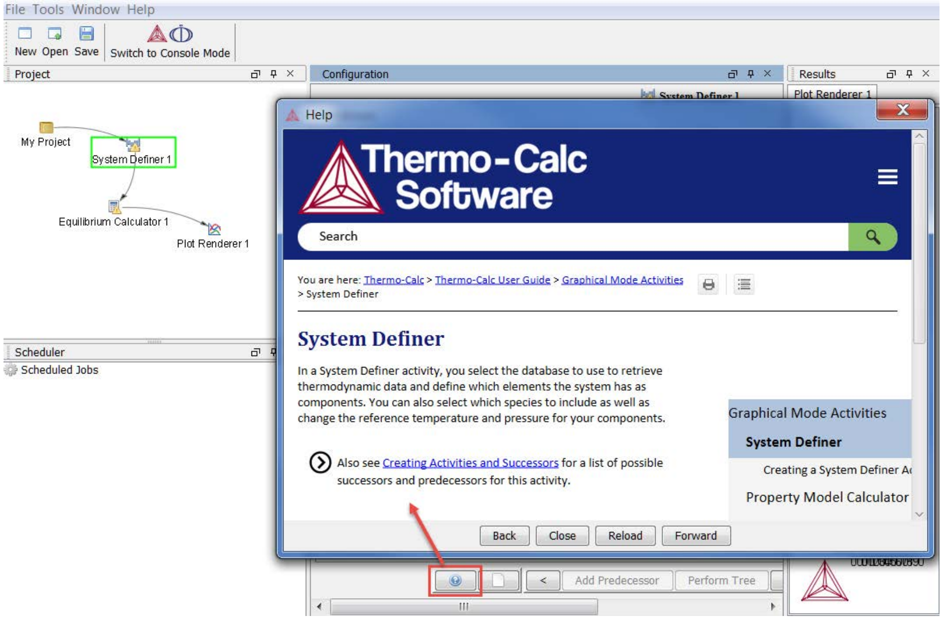
Online Help

To access online help in a browser, open Thermo-Calc and select **Help →Online Help**. The content opens in a browser but uses local content so you don't need an internet connection.

Context Help

When you are in Graphical Mode, you can access feature help (also called *topic-sensitive* or *context help*) for the activity nodes in the tree.

1. In the Project window, click a node. For example, **System Definer**.
2. In the lower left corner of the **Configuration** window, click the help button .
3. The **Help** window opens to the relevant topic.



You are here: Thermo-Calc > Thermo-Calc User Guide > Graphical Mode Activities > System Definer

System Definer

In a System Definer activity, you select the database to use to retrieve thermodynamic data and define which elements the system has as components. You can also select which species to include as well as change the reference temperature and pressure for your components.

Also see Creating Activities and Successors for a list of possible successors and predecessors for this activity.

The window that opens has the same content as the help you access in the browser. There are these extra navigation buttons in this view.

- Use the buttons on the bottom of the window, Back Close Reload Forward, to navigate **Back** and **Forward** (these are only active once you have started using the help to load pages and create a history), to **Close** the window, and **Reload** the original content.

Console Mode Help

Console Mode is for Thermo-Calc and the Diffusion Module (DICTRA).

In Console Mode at the command line prompt, you can access help in these ways:

- For a list of all the available commands in the current module, at the prompt type a question mark (`?`) and press <Enter>.
- For a description of a specific command, type `Help` followed by the name of the command. You can only get online help about a command related to the current module you are in.
- For general system information type `Information`. Specify the subject or type `?` and the available subjects are listed. This subject list is specific to the current module.

Examples, Documentation and Materials

To learn more about how to use the software you can open and run the example projects (Graphical Mode) and macro files (Console Mode). These are in the format of project files (*.TCU) and macro files (*.TCM), respectively. There are also PDF documentation sets and database information sheets included with your installation. These are also available on the Thermo-Calc Software website.

Installation Resources

On Windows, once Thermo-Calc is installed, you can also locate the Examples and Materials folders, plus all the Manuals using the shortcuts located in the Start menu. Go to **Start →** **All Programs** or **All Apps → Thermo-Calc** and click **Examples**, **Manuals**, or **Materials** as required to open the applicable folder.

In the table, <*user*> stands for the username and <*version*> for the version of Thermo-Calc, for example 2016b.

OS	**User type**	**Default directory**
Windows	Normal user	Users\<*user*>\Thermo-Calc\<*version*> Users\<*user*>\Documents\Thermo- Calc\<*version*> My documents
	Administrator	Program Files\Thermo-Calc\<*version*> Users\Public\Documents\Thermo- Calc\<*version*> Public documents
Mac	Administrator (user name and password required)	Examples and manuals in /Users/Shared/Thermo-Calc/<*version*> To go to this folder, in Finder, from the **Go** main menu select **Go to folder**. Enter the above file path and click **Go**.
Linux	Non root user	home/<*user*>/Thermo-Calc/<*version*>
	Root user	usr/local/Thermo-Calc/<*version*>

PDF Documentation

Based on your needs, there is PDF documentation available as part of your installation. These do not include the Database Information Sheets (see below).

- **Thermo-Calc Documentation Set**: Includes all the manuals needed to work with Thermo-Calc including the installation guides. For the other add-on module documentation, see the separate PDFs.
- **Installation Guides**: Includes the quick install guides for Standalone Windows and Mac installations as well as the full installation guide for all platforms and installation types.
- **Diffusion Module (DICTRA) Documentation Set**: Includes Diffusion Module (DICTRA)-specific manuals plus the Thermo-Calc User Guide, Console Mode Command Reference, Data Optimization User Guide, Database Manager User Guide, and the DATAPLOT User

Guide.

- **Precipitation Module (TC-PRISMA) User Guide**
- **SDK (Software Development Kit) Documentation Set**: Includes TQ-Interface Programmer Guide, TC Toolbox for MATLAB® Programmer Guide, and TC-API Programmer Guide.

Database Information Sheets

The database information sheets are included in the online help system and in a **Manuals** sub-folder . You can also view these on the Thermo-Calc website.

Graphical Mode Example Collection

After you have accessed the *Examples, Documentation and Materials* on page 7, go to the Graphical Mode Example folder to open one of the project files in Thermo-Calc.

Opening a Project File

Navigate to the file location and double-click the *`.tcu` file to open it. It launches a new session of the software. Or you can select **File →Open Project** from an open session of Thermo-Calc.

Also see the *Thermo-Calc Graphical Mode Examples Guide*.

The project files have the extension *`.tcu`.

Ex_01_Single-point_equilibrium.tcu
Ex_02_Step_in_temperature_in_Fe-C.tcu
Ex_03_Fe-C_phase_diagram.tcu
Ex_04_Fe-Cr-C_ternary_phase_diagram.tcu
Ex_05_Fe-C_stable_and_metastable_phase_diagram.tcu
Ex_06_Serial_equilibrium_calculators.tcu
Ex_07_User_defined_functions.tcu
Ex_08_Scheil_and_equilibrium_solidification.tcu
Ex_09_Heat_map_of_carbide_driving_force.tcu
Ex_10_Phase_Transition.tcu
Ex_11_Coarsening_and_Interfacial_energy.tcu
Ex_12_Driving_force_and_Interfacial_energy.tcu
Ex_13_Precipitation_Al-Sc_AL3SC.tcu
Ex_14_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6.tcu
Ex_15_Precipitation_Fe-C-Cr_TTT_Cementite-M7C3-M23C6.tcu
Ex_16_Precipitation_Fe-C_Cemetite.tcu
Ex_17_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime.tcu
Ex_18_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime.tcu

Examples of Thermo-Calc Activities

Example 1: Calculating a Single-Point Equilibrium

This example shows the result from a single-point equilibrium calculation in the Fe-C system. The number of equilibrium conditions is C+2 where C is the number of components, meaning that four conditions are needed in this example:

- **Temperature** is 1000 K
- **Pressure** is 101325 Pa
- **System size** is 1 mole
- **Mass percent carbon** is 0.1%

The displayed results of the calculation show that the BCC_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.

File Name	Activity Example
Ex_01_Single-point_equilibrium	Equilibrium Calculator

Example 2: Stepping in Temperature in the Fe-C System

This example shows how the fractions of stable phases vary for an Fe-0.1 mass-% C alloy when the temperature is varied between 500 and 2000 K. To allow temperature to vary, the corresponding **Axis Definition** check box is selected. In this example, results are displayed graphically using a **Plot Renderer** activity. To get text results a **Table Renderer** activity is used instead.

File Name	Activity Examples
Ex_02_Step_in_temperature_in_Fe-C	Equilibrium Calculator, Plot Renderer and a Table Renderer

Example 3: Fe-C Phase Diagrams

This example shows the stable Fe-C phase diagram (stable meaning that the graphite phase is entered in the calculation). The same diagram is calculated using a:

- **Binary Calculator** activity and a
- **System Definer** and an **Equilibrium Calculator** activity. In both cases, a **Plot Renderer** activity is used to display results. The purpose of the **Binary Calculator** is to simplify common calculations for binary systems. In the **Equilibrium Calculator** two axes are defined: *Mass percent C* and *Temperature*. An axis variable must also be an equilibrium condition.

File Name	Activity Examples
Ex_03_Fe-C_phase_diagram	Binary Calculator, System Definer and Equilibrium Calculator

Example 4: Ternary Phase Diagram in the Fe-Cr-C System at 1000 K

This example shows a ternary phase diagram in the Fe-Cr-C system at 1000 K. Similar to Example 3, the same diagram is calculated using:

- a **Ternary Calculator** activity and
- a **System Definer** and an **Equilibrium Calculator** activity. To toggle between a triangular and a rectangular diagram, press the **Show Triangular** button. To toggle the X and Y axis variables, press the **Switch Axes** button.

File Name	Activity Examples
Ex_04_Fe-Cr-C_ternary_phase_diagram	Ternary Calculator, System Definer and Equilibrium Calculator

Example 5: Stable and the Metastable Fe-C Phase Diagrams

This example shows how to overlay results from two calculations in the same plot. In *Equilibrium Calculator 1* the stable phase diagram is calculated and in *Equilibrium Calculator 2* the metastable. The Plot Renderer activity is first created as a successor to Equilibrium Calculator 1. Then right-click the Plot Renderer node and select **Add predecessor** and the results from both equilibrium calculators are in the same plot. The metastable diagram is obtained by deselecting the graphite phase in the System Definer under the **Phases and phase constitution** tab.

File Name	Activity Example
Ex_05_Fe-C_stable_and_metastable_phase_diagram	Equilibrium Calculator

Example 6: Serially Coupled Equilibrium Calculators

This example shows how to use serially coupled Equilibrium Calculators for more complex equilibrium conditions. Sometimes there are multiple possible solutions for a given set of equilibrium conditions. In other cases the equilibrium calculation does not converge. You can then aid the final calculation by, in effect, telling the software where it should start the search for the equilibrium. Here are examples of two such cases.

- In the first example, the final objective is to calculate the equilibrium at 850◦C where the mole fractions of the FCC A1 and BCC A2 phases are 0.5 each for an Fe-Cr-C steel with 10% chromium. In Equilibrium Calculator 1 a simple set of equilibrium conditions (temperature, pressure, system size and composition) are used to find a carbon content where only the FCC A1 and BCC A2 phases are stable. The results from this preliminary calculation are displayed in Table Renderer 1.

- In Equilibrium Calculator 2 the carbon content equilibrium condition is replaced by the condition that the numbers of moles of the BCC A2 phase should be 0.5. The final result is displayed in Table Renderer 2. In this case, the final objective is to calculate the solidus temperature of an Fe-Cr-C steel with 10% Cr and 0.01% C.
- In Equilibrium Calculator 3 the state at 2000 K is calculated and the result is displayed in Table Renderer 3.
- In Equilibrium Calculator 4 the temperature equilibrium condition is replaced by the condition *Fix phase / liquid / 0.0*, meaning that liquid should be stable in an amount of zero moles, i.e. the solidus temperature. The final result is displayed in Table Renderer 4.

File Name	Activity Example
Ex_06_Serial_equilibrium_calculators	Equilibrium Calculator

Example 7: User-Defined Functions

This basic example shows the use of user-defined functions. A series of equilibria for an Fe-Cr-C alloy are calculated by varying temperature between 500 and 3000 K. In the configuration window of the **Equilibrium Calculator** under the **Functions** tab, two identically meaning functions are defined, *fraction solid* and *f solid*, the values of which are plotted against temperature in the Plot Renderers. Functions can be entered in terms of *QuantitiesQ1*, *Q2*, *Q3* etc., or, for using the Thermo-Calc syntax.

File Name	Activity Example
Ex_07_User_defined_functions	Equilibrium Calculator

Example 8: Scheil and Equilibrium Solidification

This example shows a comparison for an Al-Si alloy solidified under full local equilibrium and under the Scheil assumptions, i.e. zero diffusion in the solidified material and infinitely fast diffusion in the liquid. There are three Plot Renderers created: Scheil solidification, equilibrium solidification and the third Plot Renderer includes both in the same plot.

File Name	Activity Example
Ex_08_Scheil_and_equilibrium_solidification	Scheil Calculator

Example 9: Carbide Driving Force Heat Maps

This is an example of using *property grid* calculations to plot the driving force for a carbide as a function of two composition variables. With the property grid calculation type, a 2D grid is generated from the two calculation axes. After the calculation is done, an equilibrium is calculated in each grid point. A Plot

Renderer connected to a property grid calculator plots the *z*-axis property for each equilibrium as a function of the two calculation axes. The final plot can be either a heat map or a contour plot.

File Name	Activity Example
Ex_09_Heat_map_of_carbide_driving_force	Plot Renderer

Example 10: Phase Transition

The example uses the Property Model Calculator to predict the transition temperature to the unwanted brittle Sigma phase. The example shows how the temperature is influenced by changes to a steel alloy's composition using the uncertainty calculation type and how to create either a histogram or probability plot.

File Name	Activity Example
Ex_10_Phase_Transition	Property Model Calculator

Example 11: Coarsening and Interfacial Energy

The example uses the Property Model Calculator and both thermodynamic and kinetic demonstration steel databases. Using a grid calculation type it produces three plots: a heat map, a contour plot and a cross plot with contour (where both the interfacial energy and coarsening rate is shown).

File Name	Activity Example
Ex_11_Coarsening_and_Interfacial_energy	Property Model Calculator

Example 12: Driving Force and Interfacial Energy

The example uses the Property Model Calculator and a thermodynamic demonstration steel database. Using a grid calculation type it produces a contour plot comparing the driving force and interfacial energy.

File Name	Activity Example
Ex_12_Driving_force_and_Interfacial_energy	Property Model Calculator

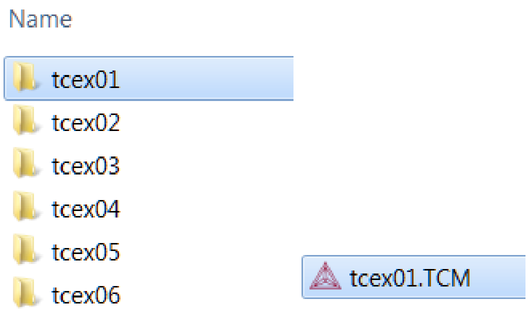
Console Mode Example Collection

After you have accessed the *Examples, Documentation and Materials* on page 7, go to the Console Mode Example folder to open one of the macro files in Thermo-Calc.

Opening a Macro File

These macro files (with the extension *.`TCM`) include comments, which you can either run in Thermo-Calc or open and read in a text editor. If you read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file.

Navigate to the file location, where each example is in its own folder.



In the folder, double-click the *.`TCM` file to open it. It launches a new session of Thermo-Calc and opens in Console Mode. If you have an instance of Thermo-Calc open in Console Mode, you can also drag and drop the file to run the macro. You can also open any text file editor and drag the file into it to see its contents.

Console Mode Example Descriptions

#	Example Description
1	Calculation of the binary Fe-C phase diagram.
2	Plotting of thermodynamic functions in unary, binary and ternary systems and working with partial derivatives and partial quantities
3	Calculation of an isothermal section using the TERNARY module.
4	Calculation of the miscibility gap in Fe-Cr
5	Calculation of a vertical section from Al to 30% Mg2Si
6	Calculation of an isopleth in low alloyed Fe-Mn-Si-Cr-Ni-C steel. This example calculates a multicomponent phase diagram using the define-material command in POLY and the TCFE steel database. The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C (by weight). These conditions and the temperature are set by the command. Hidden commands set the pressure to 1 bar and so that iron is "the rest". After calculating the first equilibrium a phase diagram is calculated with one axis variable as temperature and the other as the carbon content.
7	Calculation of single equilibria in low alloyed Fe-Mn-Si-Cr-Ni-C steel. There are two general ways to perform a single equilibrium calculation: • Get data from a database, then in POLY use SET_CONDITION and COMPUTE_EQUILIBRIUM. • Go directly to POLY and use DEFINE_MATERIAL. The COMPUTE_TRANSITION command is also used to determine the temperature or

#	Example Description
	composition where one phase forms or disappears.
8	Calculation of property diagrams for a high speed steel i.e. phase fraction plots, activity vs temperature, etc.
9	Calculation of dew point.
10	The example calculates an equilibrium with suspended or dormant phases and shows how to avoid clogging of Cr2O3 in a continuous casting process. The origin of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent but the continuous casting of this material was problematic because solid Cr2O3 was formed. Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential. In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.
11	This example demonstrates the oxidation of Cu2S with H2O/O2 gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu2S without forming copper oxides. In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu2S and H2O using a command SET_INPUT_AMOUNTS in POLY_3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.
12	This example shows a number of independent cases using the TAB- module to tabulate thermodynamic data for reactions.
13	Binary calculation of Al-Ti phase diagram and G curve.
14	Calculation of heat and heat capacity variations during solidification of an Al-Mg-Si alloy.
15	Solidification simulation of a Cr-Ni alloy using the SCHEIL module. There is no back diffusion in the solid.
16	Calculation of the second order transition line in the Bcc field of the Al-Fe system.
17	Calculation of pseudo- or quasi-binary phase diagram in the CaO-SiO2 system. This database can be used both for pseudobinary systems like the one in this case, CaO-SiO2, or for full ternary systems like Ca-Fe-O.
18	Calculation of the A3 temperature of a steel and the influence of each alloying element on this temperature.

#	Example Description
	A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. But for complex multicomponent steels, no simple diagram can be used. This example shows how to calculate the A3 temperature of a steel. Using POLY, it is easy to find out the influence of each alloying element on A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.
19A	Mapping of univariant equilibria with the liquid in Al-Cu-Si. Part A. Step-by-step calculation using POLY.
19B	Mapping of univariant equilibria with the liquid in Al-Cu-Si. Part B. Using the TERNARY module, you can get the information on invariant reactions, such as temperature and compositions.
20	Calculation of adiabatic decompression in a geological system using the geochemical database.
21	Calculate a ternary isotherm in Fe-Cr-Ni with a user-defined database.
22	Calculation of a heat balance. In this case C3H8 is burned in oxygen and the adiabatic flame temperature is calculated.
23	Calculation of a para-equilibrium and the T0 temperature in a low alloyed steel.
24	Simulation of the silicon arc furnace using the REACTOR module. This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80 % reacts in the first above, 15% in the second above and 5 % in the third above. The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify their heat content.
25	Simulation of steel refining. Raw iron used to produce steel usually has high carbon and silicon content, which is why oxygen is blown into the furnace to burn off carbon. Lime (CaO) is added to form a slag with silica, and the slag can be removed. Alloying elements, such as Mn, Ni, Cr and V are added to produce the desired steel. Since the reaction between O and C increases the temperature, scrap iron is added in order to keep the temperature constant (it is assumed the furnace is isolated and no heat is lost to the environment). This is a typical steel refining process. This example simulates blowing oxygen into a liquid steel of one metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant is the way to simulate the isolation of the furnace. The oxygen reacts with carbon and increases the temperature. After blowing a certain amount of oxygen, scrap iron is added to keep the temperature constant.

#	Example Description
26	Example of plotting the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid AsGa.
27	CVD calculations
28	Example showing calculation of PRE (Pitting Resistance Equivalence) for a duplex stainless steel.
29	Calculation of speciation of a gas
30A	Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy. Part A. Step-by-step calculation using POLY and the STEP_WITH_OPTION command, EVALUATE option.
30B	Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy. Part B. Simulation performed using SCHEIL module.
31	Calculations of CVM and comparisons with sublattices of a fictitious A B system. Also shows how to overlay diagrams from two calculations.
32	Calculation of oxide layers on steel. Also shows how to append databases.
33	Benchmark calculation - An isopleth in the Fe-Cr-C system.
34	Calculation of the phase diagram and G curves in the Al-Zn system. An example of using the BINARY module.
35	Calculation of potential diagram
36	Assessment - The use of the PARROT module The example is divided into four parts corresponding to the files in the folder. The problem is presented with "selected" experimental data (see the *tcex.36.readme* file). The example uses a fictitious binary A-B system where element A is BCC until it melts. Element B is BCC up to 1100 K and FCC above. There is a compound A2B stable in a limited temperature range. • The creation of the "setup" file is described (*tcex36a.TCM*) • The creation of the experimental data file is described (*tcex 36b.TCM*) • The actual run in the PARROT module in order to obtain the result (*tcex 36cp-d.TCM*)
37	Calculation of an isothermal section using command lines.
38	Calculation of the Morral “rose” (miscibility gaps).

#	**Example Description**
39	This example shows how Thermo-Calc calculates the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2. The Reversible Carnot cycles are usually drawn schematically. Using Thermo-Calc and realistic data it is possible to calculate a reversible Carnot cycle of a heat engine and to relate it to different thermodynamic quantities. One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve.
40	A series of examples designed to demonstrate the advanced POURBAIX module calculations and graphical processing. Also see the text file the Extended folder (*TCEX40-README.txt*). The first example automatically calculates and plots a Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at 25C and 1 bar. A so-called Pourbaix diagram is actually a phase diagram with independently-varied acidity (pH) and electropotential (Eh), for a heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water dissolving a specified amount of metals and other solutes), under a defined temperature and pressure condition. For details about the other examples, see *Pourbaix Examples TCEX40, 40A to 40E, and TCEX53* on page 170.
41	Calculation of a solubility product. Shows the STEP_WITH_OPTION command, T-ZERO option.
42	Formation of para-pearlite (isopleth calculation) Fe-Mn-C system at 2.5%Mn Mass u-fraction (an example of a paraequilibrium calculation).
43	Formation of para-pearlite (calculation of isothermal section) Fe-Mn-C system at 700 C (an example of a paraequilibrium calculation).
44	This example uses variables and functions to predict properties e.g. proof strength for an austenitic stainless steel at elevated temperatures (20-550C). The example was created using an expression from Eliasson, Johan, and Rolf Sandström. "Proof strength values for austenitic stainless steels at elevated temperatures." *Steel research* v. 71, no. 6-7 (2000): 249-254.
45	3D-diagram that calculates the gamma volume in the Fe-Cr-C system. To view the generated file, *tcex45.wrl*, install a WRML (Wirtual Reality Modelling Language) viewer to the web browser. WRML viewers can be downloaded from various sites, e.g. www.parallelgraphics.com or www.sim.no.
46	3D-diagram that calculates the liquidus surface of the Fe-Cr-C system.

#	Example Description
	To view the generated file, *tcex46_tri.wrl* and *tcex46_sqrt*, install a WRML (Wirtual Reality Modelling Language) viewer to the web browser. WRML viewers can be downloaded from various sites, e.g. www.parallelgraphics.com or www.sim.no..
47	3D-quaternary diagram that calculates the gamma volume in the Fe-Cr-V-C system at 1373K. To view the generated file, *tcex47.wrl*, install a WRML (Wirtual Reality Modelling Language) viewer to the web browser. WRML viewers can be downloaded from various sites, e.g. www.parallelgraphics.com or www.sim.no..
48	This is an example of Scheil solidification with C back diffusion in solid phases and compares it with simple Scheil and equilibrium calculations.
49	This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS_ENERGY_SYSTEM (GES) module commands.
50	This example shows the quasichemical model using TDB to replicate figures 3 and 4 from Kongoli, F., Pelton, A. D. & Dessureault, Y. Thermodynamic modeling of liquid Fe-Ni-Cu-Co-S mattes. *Metall. Mater. Trans. B* 29, 591–601 (1998).
51	Calculation of molar volume, thermal expansivity and density.
52	This example shows how to change the excess models for binary/ternary interactions in a solution phase, either through direct interactive amendments of phase descriptions within the GIBBS_ENERGY_SYSTEM (GES) module, or enforced by specific type-definitions given in a database file retrieved by the TDB module. For binary excess model: from the default R-K model to Mixed-Excess-Model (Note the phase has to be a substitutional phase) For Ternary Extrapolation Model: from the default R-K-M model to Toop_Kohler model.
53	Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine. Using PAQ2 or PAQS2 database; for the Fe-X-H2O-NaCl heterogeneous interaction systems (X = Cr-Ni-Co).

The Thermo-Calc Modules and Activities

Although many calculations can be done in either Graphical or Console Mode, only data optimization and thermodynamic or kinetic assessments are available in Console Mode. Conversely, only the Property Model Calculator is available in Graphical Mode.

For the Console Mode only commands see *The Console Mode Interface* on page 113 and the *Thermo-Calc Console Mode Command Reference* included with this documentation set.

Modules and Activities briefly describes the available modules. The specific modules, using the names in the table, are accessed through Console Mode. For Graphical Mode, the underlying principles, and the final calculations, are incorporated into the projects and activities. Some modules require additional licenses.

Modules and Activities

The first and second columns are the Console Mode module names. The third column indicates whether there is an equivalent activity available in Graphical mode.

Full Module Name in Console Mode	**Short Name**	**Graphical Mode Activity**	**Primary Functions**
BINARY_ DIAGRAM_EASY	BIN	*Binary Calculator* on page 105	Calculate binary phase diagrams. Access to specific databases designed for BIN, such as TCBIN, is required.
DATABASE_ RETRIEVAL	DATA	*System Definer* on page 55	Select appropriate databases, define chemical systems and retrieve the data required for calculations.
DICTRA_ MONITOR	DICTRA	Console Mode only	Run simulations of diffusion controlled transformations in Thermo-Calc using the Diffusion Module (DICTRA). An additional license is required for this feature.
DIC_PARROT	DIC_PARROT	Console Mode only	This is the data optimization module for the Diffusion Module (DICTRA). It allows you to assess experimental data and use such data to optimize calculations. An additional license is required for this feature.
EDIT_ EXPERIMENTS	ED_EXP	Console Mode only	Part of the PARROT submodule, use it to edit experimental data points to make reliable optimizations.
GIBBS_ENERGY_ SYSTEM	GIBBS	Console Mode only	Handles thermodynamic models and quantities. Generally you do not need to use this module, but you can get information about models, and list, add or amend the thermodynamic parameters in use.

Full Module Name in Console Mode	**Short Name**	**Graphical Mode Activity**	**Primary Functions**
PARROT	PARROT	Console Mode only	A data optimization module to assess experimental data and use the data to optimize calculations.
not available	-	*Precipitation Calculator* on page 79	Set the conditions for, and perform, a precipitation calculation.
not available	-	*Property Model Calculator* on page 61	You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot.
POLY-3	POLY	*Equilibrium Calculator* on page 73	Equilibrium calculation module. Specify conditions and make calculations.
POST_ PROCESSOR	POST	*Plot Renderer* on page 84	For post-processing and plotting of calculation results. Modify property and phase diagrams, add labels, change the diagram colours, etc. Submodules to POLY-3 and DICTRA module for example.
POTENTIAL_ DIAGRAM	POTENTIAL	*Ternary Calculator* on page 107	Calculate and plot gas potential diagrams in a ternary system. The potential of two gas species are used as the diagram axes.
POURBAIX_ DIAGRAM	POURBAIX	Console Mode only	Calculate and plot pH-Eh diagrams (Pourbaix diagrams) and property diagrams for heterogeneous interaction systems involving aqueous solutions.
REACTOR_ SIMULATOR_3	REACTOR	Console Mode only	Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.
SCHEIL_ SIMULATION	SCHEIL	*Scheil Calculator* on page 109	Simulate and plot Scheil-Gulliver solidification processes with no diffusion in the solid phases and with/without consideration of back diffusion of interstitial components (such as C, N, O, S).

Full Module Name in Console Mode	**Short Name**	**Graphical Mode Activity**	**Primary Functions**
SYSTEM_ UTILITIES	SYS	Console Mode only	In Console Mode, interact with the operating system and change environmental settings. Create and execute MACRO files.
TABULATE_ REACTION	TAB	Console Mode only	Tabulate properties of chemical reactions and substances (stoichiometric or solution phases).
TERNARY_ DIAGRAM	TERN	*Ternary Calculator* on page 107	Calculate ternary phase diagrams.

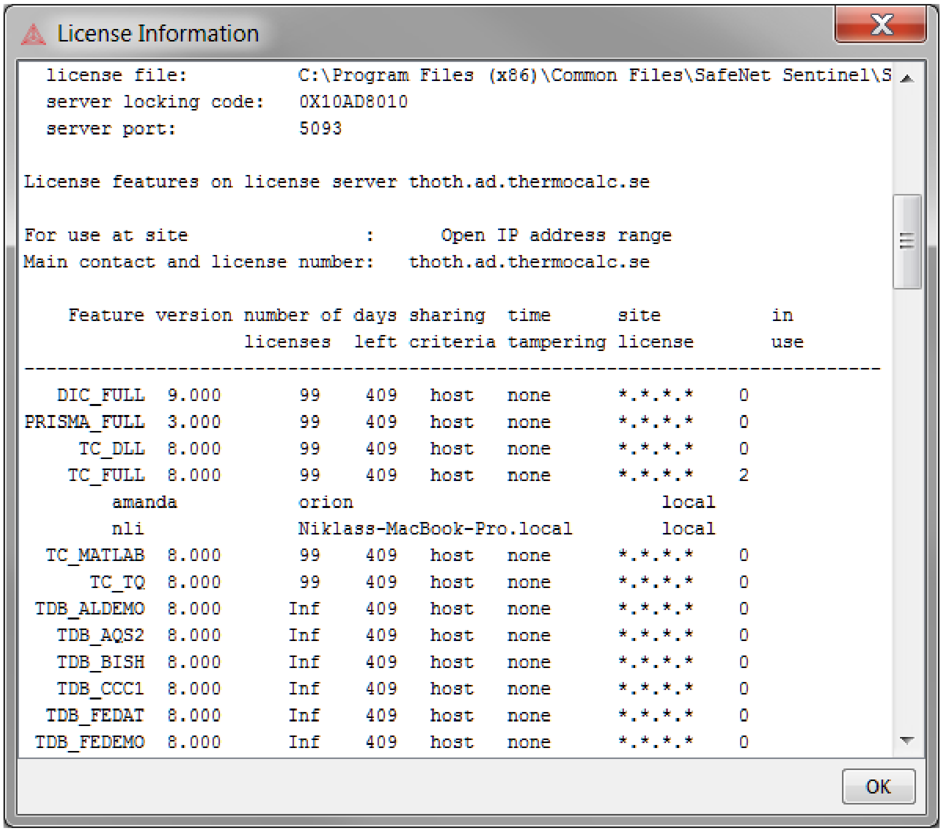
Displaying Thermo-Calc License Information

You can start (and install) the software without a valid Thermo-Calc license but you cannot do any calculations. To show information about the available and installed licenses, from the main menu select **Help → Show License Info**.

Also see the *Thermo-Calc Installation Guide*.

License Information Window Example

This is an example of part of a License Information window for a network installation.



```
  license file:          C:\Program Files (x86)\Common Files\SafeNet Sentinel\S
  server locking code:   0X10AD8010
  server port:           5093

License features on license server thoth.ad.thermocalc.se

For use at site                :      Open IP address range
Main contact and license number:   thoth.ad.thermocalc.se

    Feature version number of days sharing  time      site          in
                    licenses  left criteria tampering license       use
------------------------------------------------------------------------------
   DIC_FULL  9.000       99    409   host   none      *.*.*.*    0
PRISMA_FULL  3.000       99    409   host   none      *.*.*.*    0
     TC_DLL  8.000       99    409   host   none      *.*.*.*    0
    TC_FULL  8.000       99    409   host   none      *.*.*.*    2
        amanda           orion                            local
        nli              Niklass-MacBook-Pro.local        local
  TC_MATLAB  8.000       99    409   host   none      *.*.*.*    0
      TC_TQ  8.000       99    409   host   none      *.*.*.*    0
 TDB_ALDEMO  8.000      Inf    409   host   none      *.*.*.*    0
   TDB_AQS2  8.000      Inf    409   host   none      *.*.*.*    0
   TDB_BISH  8.000      Inf    409   host   none      *.*.*.*    0
   TDB_CCC1  8.000      Inf    409   host   none      *.*.*.*    0
  TDB_FEDAT  8.000      Inf    409   host   none      *.*.*.*    0
 TDB_FEDEMO  8.000      Inf    409   host   none      *.*.*.*    0
```

Under each license type with instances checked out, there is a list of who checked out each license. In Graphical Mode, an instance is checked out when an Equilibrium Calculator activity is created, and checked back in when that Equilibrium Calculator is removed. In Console Mode, an instance is checked out when you enter the POLY module and is checked back in when you exit the POLY module. In the example, two users, amanda and nli, have licenses checked out.

- The **Features** column is a list of the specific software, databases and API licenses purchases.
- The **Version** is an internal version number for the feature.
- The **number of licenses** column is how many instances of each license type available to be checked out simultaneously.
- The **in use** column shows how many license instances are checked out.

Console Mode License Restrictions

- If you start Thermo-Calc without a valid Thermo-Calc license you cannot leave the SYS module.
- If all the licenses are checked out for a network client installation of Thermo-Calc, you may not be able to enter the POLY or DICTRA modules until a license is available.

- To enter the DICTRA and the DIC_PARROT modules, you need a valid Diffusion Module (DICTRA) license key.
- If you enter and use either the DIC_PARROT module or the PARROT module, then you cannot enter the other module in the same session. You must close down Thermo-Calc and launch the program again to enter the other data optimization module.

Network Computer License Restriction

If you have a network computer installation of Thermo-Calc, then you may not be able to do any calculations even if you have access to a valid network license file. This is because others who are part of your network installation may have checked out all allowed instances of the software.

If you are running a network installation of Thermo-Calc, you can see how many instances of the client licenses are currently checked out and how many of them are left. You can also see which client computers have checked out the licenses.

Using This Guide

If you are a new user, Graphical Mode is a good way to learn how to work with Thermo-Calc. Console Mode has more functionality but until you are comfortable with the concepts, it is recommended you start in Graphical Mode.

Additional documentation and training material is described in *Help Resources* on page 5.

Graphical Mode

The Graphical Mode Interface on page 27 introduces you to the GUI layout and the workflow. In *Graphical Mode Projects* on page 43, it goes into more detail about how to set up and run your projects (with the Quick Start Wizard), using templates, scheduling jobs and creating activities. *Graphical Mode Activities* on page 54 specifically describes how to set up each type of available activity in the tree structure.

For both Graphical and Console mode, *Changing Global Settings* on page 189 gives information about adjusting global user settings.

Console Mode

Console Mode has more functionality than Graphical Mode but the underlying concepts are the same. There are, however, command lines and extensive details applicable to this mode. This guide is only the beginning of the learning objectives. In particular, refer to the *Thermo-Calc Console Mode Command Reference* for details about all the commands available.

In this guide it is a basic introduction to the layout of the Command windows, as described in *The Console Mode Interface* on page 113.

Several topics describe and give an example of the calculation types:

- *Equilibrium Calculations* on page 132
- *Property Diagrams* on page 138
- *Phase Diagrams* on page 142
- *Scheil Simulations* on page 146
- *T0 Temperature Simulations* on page 152
- *Paraequilibrium* on page 155
- *Potential Diagrams* on page 159
- *Aqueous Solutions* on page 163
- *Console Mode TAB Module* on page 176

Then in *Console Mode POST Module* on page 181 there is an overview of plotting.

For both Graphical and Console mode, *Changing Global Settings* on page 189 gives information about adjusting global user settings.

The Graphical Mode Interface

These topics introduce you to the concepts and terminology of Graphical Mode and describe the basic workflow.

In this section:

The GUI Layout

Open Thermo-Calc to view the default GUI layout for Graphical Mode. You can easily reorganize the windows.

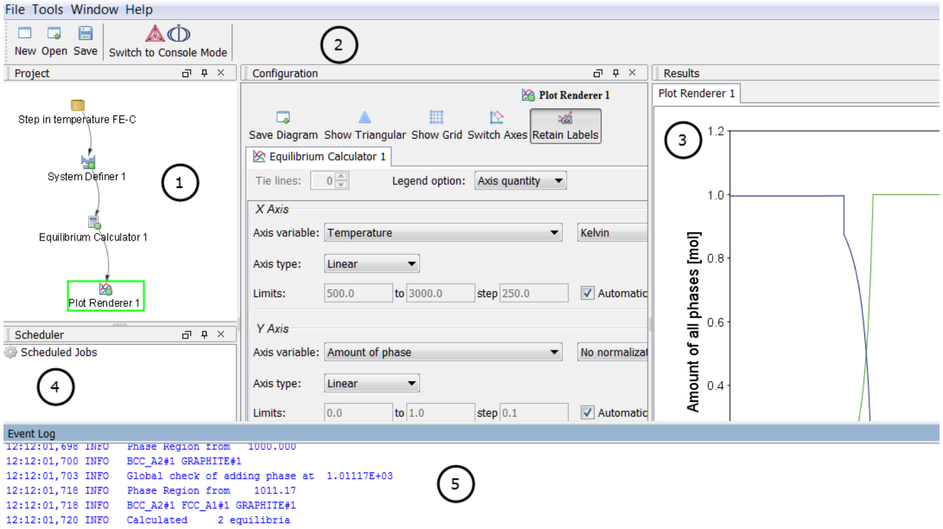
Also see *Moving Windows* on page 39.

The windows are:

1. **Project**: Create, manipulate and navigate between the activities that make up a project.
2. **Configuration**: Shows the settings that can be configured for the currently selected activity.
3. **Results**: Shows the results of a calculation, either plotted as a diagram or displayed in table format. In this example, there is a Plot Renderer *tab* in the Results window.
4. **Scheduler**: Displays information about jobs, such as calculations, that are being performed or are scheduled to be performed. You can cancel scheduled jobs and if a job has failed, then you can view information about the error.
5. **Event Log**: By default this window is closed but it displays during calculation processes. You can always open it to view progress of calculations and to troubleshoot.

Graphical Mode Windows

In this example, the Results window also has a Plot Renderer tab. You can also have a Table Renderer tab.



Tie lines: 0
Legend option: Axis quantity

X Axis
Axis variable: Temperature
Kelvin
Axis type: Linear
Limits: 500.0 to 3000.0 step 250.0
☑ Automatic

Y Axis
Axis variable: Amount of phase
No normalizat
Axis type: Linear
Limits: 0.0 to 1.0 step 0.1
☑ Automatic

```
12:12:01,698 INFO   Phase Region from   1000.000
12:12:01,700 INFO   BCC_A2#1 GRAPHITE#1
12:12:01,703 INFO   Global check of adding phase at  1.01117E+03
12:12:01,718 INFO   Phase Region from    1011.17
12:12:01,718 INFO   BCC_A2#1 FCC_A1#1 GRAPHITE#1
12:12:01,720 INFO   Calculated     2 equilibria
```

Project Activities and the Tree Structure

In a *project*, a set of linked activities is called a *tree*. A result calculated within a tree is fed as input into the next *activity* in the tree. Consequently, if you have an Equilibrium Calculator with another Equilibrium Calculator as its *successor*, the successor takes the calculation results of the *predecessor* as the starting values for its calculation. When working with activities in the Project window these are also referred to as *nodes* (or *activity nodes*) in the tree structure.

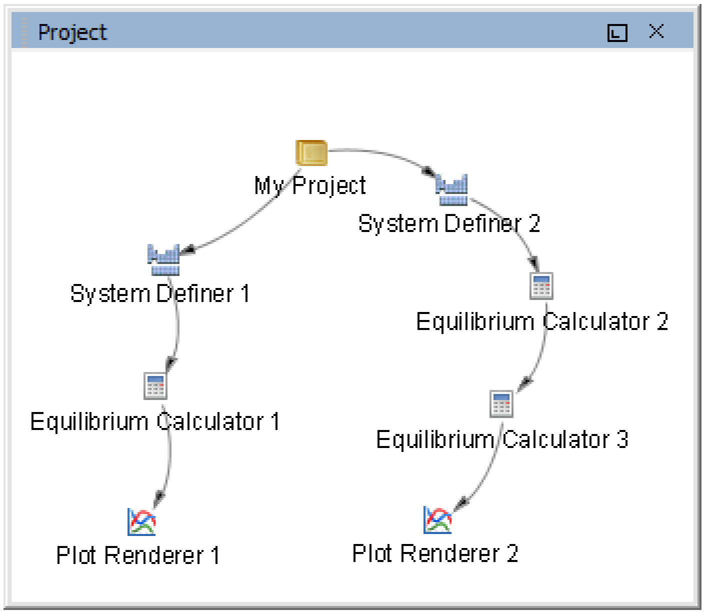
Also see *Activity Successor and Predecessor Nodes* below for definitions.

The **Project Tree Example** shows a My Project node with two trees. In each tree, settings and calculation results are propagated downward until the calculation and the visualisation of the results are completed in the Plot Renderer nodes.

The system definitions, settings and calculation results of the two trees are independent of each other.

Project Tree Example

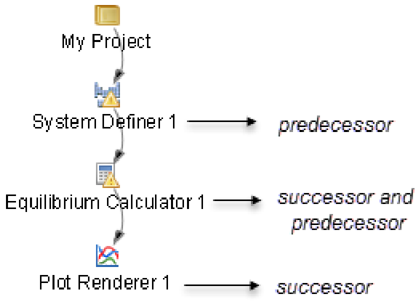
Project window with a My Project node. There are two trees with successor and predecessor activity nodes.



Activity Successor and Predecessor Nodes

An activity node located below another activity node in a tree is referred to as that activity's *successor*. An activity located above another activity is called that activity's *predecessor*. A predecessor is performed before the predecessor's successors and its result is fed forward to any successor activities.

Example of the Tree Structure



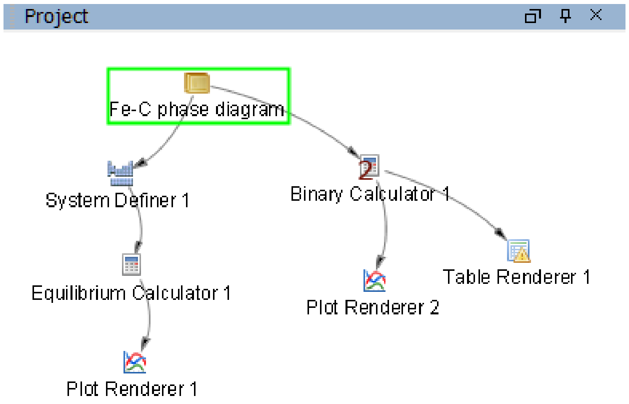
For example, to calculate and display a phase diagram, create a branch with three linked activities: A System Definer activity linked to an Equilibrium Calculator activity, which in turn is connected to a Plot Renderer activity.

See *Successor and Predecessor Example* below, which shows that Binary Calculator 1 is a predecessor to the successors, Plot Renderer 2 and Table Render 1.

You can determine the available successors by right-clicking a node in the Project window and choosing options from the menus.

Also see *Creating Activities and Successors* below.

Successor and Predecessor Example



Creating Activities and Successors

You can create a new activity in these ways:

- In the **Project** window, right-click an activity and choose **Create New Activity** (**My Project** node only) or **Create New Successor** (all other nodes).
- Select the activity you want to create from the submenu.

- At the bottom of the **Configuration** window, click **Create New Activity** or **Create New Successor** and select the activity to create.

Predecessors and Successors by Activity

Activity	Possible Predecessors	Possible Successors
My Project	None; this is the first node of the tree structure	System Definer, Binary Calculator, Ternary Calculator, Experimental File Reader. Also choose templates from this level.
System Definer on page 55	My Project, System Definer	Property Model Calculator, Equilibrium Calculator, Precipitation Calculator, Scheil Calculator
Property Model Calculator on page 61	System Definer	Plot Renderer
Equilibrium Calculator on page 73	System Definer, Equilibrium Calculator	Equilibrium Calculator, Plot Renderer, Table Renderer
Precipitation Calculator on page 79	System Definer	Plot Renderer, Table Renderer
Plot Renderer on page 84	Property Model Calculator, Equilibrium Calculator, Precipitation Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator, Experimental File Reader	None
Table Renderer on page 102	Equilibrium Calculator, Precipitation Calculator, Binary Calculator, Scheil Calculator	None
Experimental File Reader on page 105	My Project	Plot Renderer
Binary Calculator on page 105	My Project	Plot Renderer, Table Renderer
Ternary Calculator on page 107	My Project	Plot Renderer
Scheil Calculator on page 109	System Definer	Plot Renderer, Table Renderer

Graphical Mode Workflow

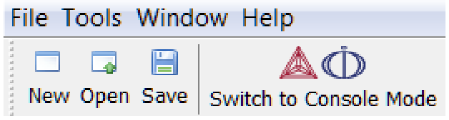
You can set up a tree in the Project window (starting with the My Project node) and then perform all the activities at once, or create and perform one activity at a time.

The typical workflow is to:

1. *Define a System*: Create a *System Definer* on page 55 activity (in the **Project** window) where you select a database and the elements to have as system components (in the **Configuration** window).
2. *Set up and run a calculation*: Create an *Equilibrium Calculator* on page 73 activity (a successor to the **System Definer**), where calculation conditions are set (temperature, pressure, etc.). This is where axis variables are set to create a property or phase diagram. These settings are also made in the **Configuration** window. You can also create a *Property Model Calculator* on page 61, *Precipitation Calculator* on page 79 or *Scheil Calculator* on page 109.
3. *Visualize the results*: Create either a *Plot Renderer* on page 84 or a *Table Renderer* on page 102 activity in the **Project** window. When calculated, this creates a plot or table in the **Results** window. The results are shown in a **Plot Renderer** or a **Table Renderer** tab.

You need to Perform a Plot Renderer or a Table Renderer activity to visualize the calculation results from an Equilibrium Calculator.

Main Menu and Toolbar



Graphical Mode Menu and Toolbar Options lists the main menu and toolbar options. The **File** menu and toolbar are reserved for Graphical Mode but in Console Mode the **Tools**, **Window** and **Help** menus have the same options.

In Console Mode you use commands to access the other options instead. These are discussed in *The Console Mode Interface* on page 113.

Graphical Mode Menu and Toolbar Options

Option	Description	Action (s)
New	Create a new project.	Click **New** on the toolbar Select **File** → **New Project** Press <Ctrl+N>
Open	Open an existing project. See *Saving and Opening Thermo-Calc Project Files* on page 35.	Click **Open** on the toolbar Select **File** → **Open Project**

Option	**Description**	**Action (s)**
		Press <Ctrl+O>.
Save	Save a project. See *Saving and Opening Thermo-Calc Project Files* on the next page.	Click **Save** on the toolbar Select **File → Save Project** Press <Ctrl+S>.
Switch to Console Mode	Launch Console Mode and the command prompt.	Click the button to exit Graphical Mode and open Console Mode.
Switch to Graphical Mode	Launch Graphical Mode to work with the GUI version.	Click the button to exit Console Mode and open Graphical Mode.
Append Project	Combine two projects into one project file. See *Saving and Opening Thermo-Calc Project Files* on the next page.	Select **File → Append Project**
Save Project As...	Save an existing project with a new name.	Select **File → Save Project As...**
Exit	Exit the program.	In the upper right-corner of the program, click the X. Select **File → Exit** Press <Ctrl+Q>.
Options	Change the global defaults for a variety of settings. See *Changing Global Settings* on page 189.	Select **Tools → Options**
Database Checker	Open the Database Checker, a program to check that the syntax of Thermo-Calc database files is correct. This is for advanced users who develop and manage databases.	Select **Tools → Database Checker**
Window menu	Highlight a specific window on the GUI	From the **Window** menu, select an option to refocus on that specific window.
Online Help	Open the online help system where you can browse or search all the Thermo-Calc documentation.	Select **Help → Online Help**
Show License Info	Open the License Information window.	Select **Help → Show License Info**

Option	Description	Action (s)
	Also see *Displaying Thermo-Calc License Information* on page 23 and in the *Thermo-Calc Installation Guide* .	
Check for update	Check the Thermo-Calc Software website for updates to the software.	Select **Help → Check for update**

Saving and Opening Thermo-Calc Project Files

Thermo-Calc Graphical Mode uses project files with the file name suffix `.TCU`.

To save your project and all its settings and results, on the toolbar click **Save**. Select to **Include calculated results in the project file** (the default) as required.

To open a Thermo-Calc project file, on the toolbar click **Open** and select the project file in the **Open file** window.

You can only have one project file open at a time. However, you can attach (*append*) the trees from additional project files to the topmost My Project node. To append an additional project file in this way, from the main menu select **File → Append Project** and open a project file.

Also see *Saving Plots* on page 96 and *Saving Tabulated Data* for the *Table Renderer* on page 102.

Project Activity Nodes

Project Activity Node Descriptions is a brief description of the project activity types. When working with activities in the Project window these are also referred to as nodes.

Project Activity Node Descriptions

These are the project activity nodes available in Graphical Mode.

Activity type	**Description**
System Definer on page 55	Define a certain thermodynamic system and read it from file into memory.
Property Model Calculator on page 61	Choose one or more general models to predict and optimize material properties. You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot.
Equilibrium Calculator on page 73	Set thermodynamic conditions and define axis variables when a series of equilibrium calculations are to be performed in one or more dimensions.
Precipitation Calculator on page 79	Set the conditions for, and perform, a precipitation calculation.
Plot Renderer on page 84	Determine the layout of non-text based output.
Table Renderer on page 102	Use it for text-based output.
Binary Calculator on page 105	Use it for some calculations involving two components only. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on binary systems. To perform this activity, you need a database designed for the Binary Calculator, such as the TCBIN database.
Ternary Calculator on page 107	Use it for some calculations involving three components. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on ternary systems. To get a reliable result you need a database that fully assesses binary and ternary systems.
Scheil Calculator on page 109	Perform Scheil-Gulliver calculations (also known as Scheil calculations). A default Scheil calculation is used to estimate the solidification range of an alloy assuming that i) the liquid phase is homogeneous at all times and ii) the diffusivity is zero in the solid. However, it is possible to disregard the second assumption for selected components.
Experimental File Reader on page 105	Read experimental data files (*.EXP). This type of file contains information specifying a plotted diagram, written in the DATAPLOT graphical language.

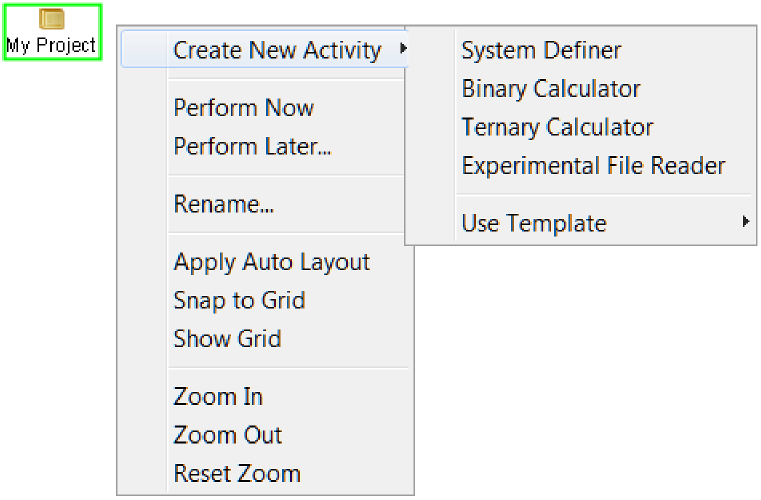
Activity type	Description
	Also see the *DATPLOT User Guide*.

Project and Activity Menus

When working in the Project window you can right-click nodes to open menus with the available actions. For example, click the **My Project** node to open the menus.

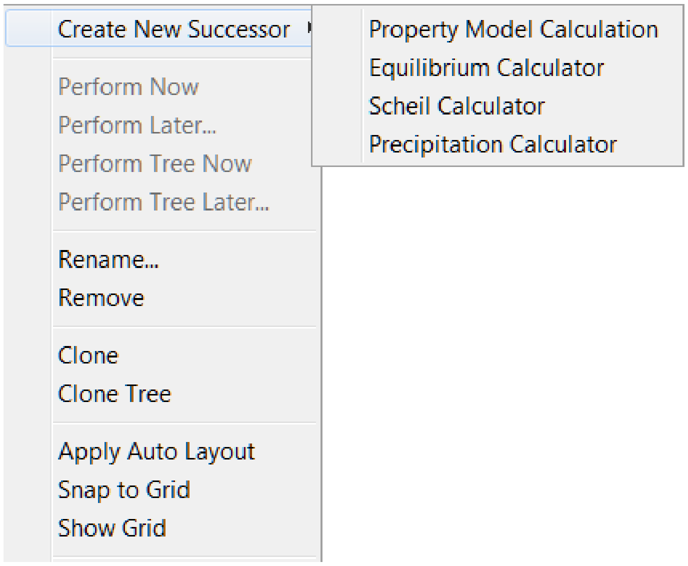
My Project Node

Menu options available for My Project node.



Activity Node Menu Example

Most nodes in the tree have a common menu with differences due to placement in the tree and the activity type.



Menu Options for Activities

Option	Description	Action (s)
Create New Activity	Add System Definer, Binary Calculator, Ternary Calculator, and Experimental File Reader nodes. See *Creating Activities and Successors* on page 30.	Right-click **My Project** and from the **Create New Activity** menu choose an option.
Create New Activity → Use Template	Choose from the available templates to use the Wizard or add predefined nodes. See *Creating a Project from a Template* on page 47.	Right-click **My Project** and from the **Create New Activity→ Use Templates** menu choose an option. The templates are also available on the **Configuration** window, which you can access by clicking the **My Project** node, or from the **Window** menu.
Create New Successor	Add a successor to the selected node. See *Creating Activities and Successors* on page 30.	Right-click one of these nodes **System Definer**, **Property Model Calculator**, **Equilibrium Calculator**, **PRISM Calculator**, **Binary Calculator**, **Ternary Calculator** or **Experimental File Reader**, and from the **Create New Successor** menu choose an option.

Option	Description	Action (s)
Add a Predecessor	Add a predecessor to the selected node.	Right-click a node to add a predecessor to it (when available).
Perform Now or Perform Later	Perform a calculation or create a plot or table immediately, or schedule it for a time in the future. See *Using the Scheduler* on page 50.	Right-click any node.
Rename	Change the name of the node.	Right-click any node.
Remove	Delete the selected node from the tree.	Right-click any node except My Project.
Clone	Duplicate the selected node and add it to the same tree. See *Cloning Activities and Trees* on page 48.	Right-click any node except My Project.
Clone tree	Duplicate a tree and add it to My project.	Right-click any node except My Project.
Apply Auto Layout	Apply an automatic layout to the nodes in the tree.	Right-click any node.
Snap to Grid	Snap a node to align it with the grid. See *Moving Nodes in the Tree and Using the Grid* on the next page.	Right-click any node.
Show Grid	Turn the grid on or off in the Project window.	Right-click any node.
Zoom In, Zoom Out, Reset Zoom	Zoom in and out of the Project window or reset the zoom to the default.	Right-click any node.

Moving Windows

The windows in Thermo-Calc can be fixed or free-floating. When fixed, it can also be set to auto-hide, where the window is minimized if you select another window. The minimized window is then shown either along the bottom or side of the Thermo-Calc window. A free-floating window is shown on top of the other windows and can be moved outside the frame of the Thermo-Calc window.

By default, the windows are fixed and open, except the **Event Log** window, which is set to auto-hide by default.

To return to the standard desktop layout, from the main menu, select **Windows** → **Reset Windows**.

Floating, Hiding and Minimizing Windows in the GUI

For each window you can rearrange, resize, minimize and close it. At the top right corner are the buttons listed in the table.

Button(s)	Description
🗗 🗖	Click to toggle on/off free-floating
📌 ⊣	Click to toggle on/off auto-hide.
–	Click to minimize an open window that has auto-hide turned on. The window automatically minimizes if another window is selected.
×	Click to close the window. You can open the window again from the Window main menu.

Moving Nodes in the Tree and Using the Grid

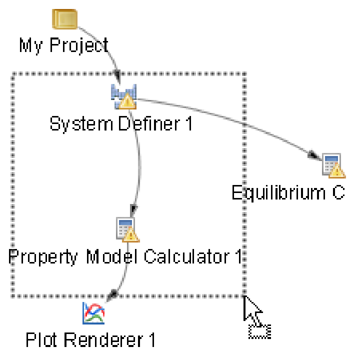
In the Project window, you can work with the activity nodes in these ways.

Select and Move Individual Nodes

- Click an activity node to *select* it.
- To move activities, click and hold the activity node and move the cursor.

Select Several Nodes at a Time

- To select several activity nodes, hold down <Ctrl> while clicking on each node you want to select.
- Click and hold the mouse button and draw a square around the activity nodes to select. Both the name and the icon that represents an activity must be within the square.



Zoom In and Out

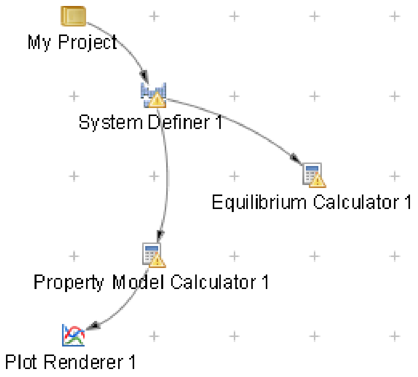
- Zoom in and out with the mouse scroll wheel.
- In the **Project** window right-click and select **Zoom In** or **Zoom Out**. To go back to the default zoom, select **Reset Zoom**.

Show Grid and Snap to Grid

To show a grid of light-grey cross-hairs overlaid on a project, click **Show Grid** in the toolbar. Click the button again to turn the grid off. Or right-click in the **Project** window and select **Show Grid**.

Click **Snap to Grid** in the toolbar or right-click in the **Project** window and select **Snap to Grid** to automatically position each activity in the Project window at a cross-hairs point in the grid.

The Project window with the grid turned on and activity nodes moved from the default location. These nodes are snapped to the grid.



Node Status Markers

Status markers indicate whether an activity is ready to be performed, is being performed, or has been performed. The markers are overlaid on the activity icons in the **Project** window. The status markers are displayed on a System Definer icon.

Node Status Markers for the Project and Scheduler Windows

Window	Status marker	Description
Project window		No status marker means the activity is ready to be performed (it has not been performed).
	⚠	A yellow triangle means the activity cannot be run. The necessary configurations for the activity may not be set or other prerequisites are not met.
	🟢	A green disc means the activity is performed.
	⏰	A red circle with a dial (a clock face) means the activity is currently being performed.
Scheduler window		No status marker means the activity (the job) is scheduled to be performed (the job has not started).
	⚠	A yellow triangle means there an error happened during the activity job.
	🟢	A green disc means the activity (the job) performed successfully.
	➡	A green right-facing arrow means the activity (the job) is being performed.

Graphical Mode Projects

These topics describes how you create, perform and link activities.

In this section:

The Quick Start Wizard

Even before you understand how to work with Thermo-Calc projects, the Quick Start wizard helps you set up a project and run calculations in Graphical Mode. You can set up, calculate and visualize any of the following:

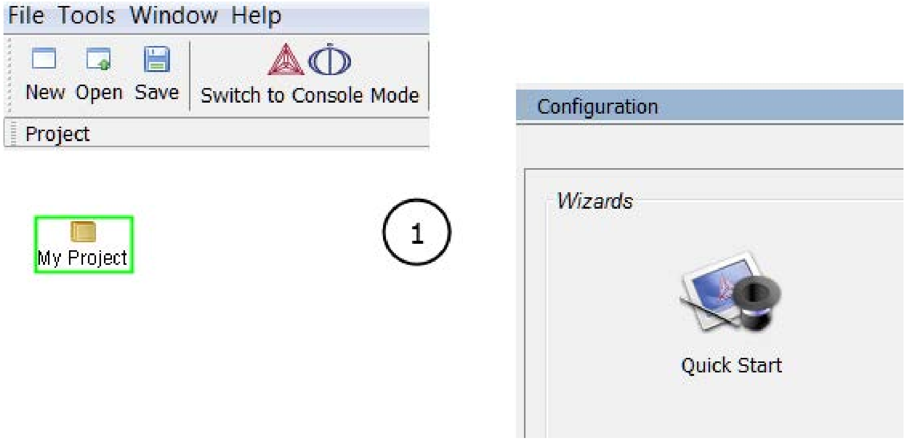
- Single point equilibrium
- Property diagram
- Phase diagram
- Scheil solidification simulation

See *Creating a Project with the Quick Start Wizard* below

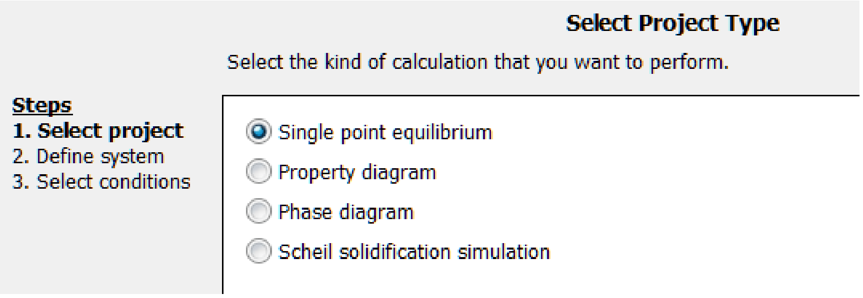
Creating a Project with the Quick Start Wizard

To set up, perform and visualize a calculation using the Quick Start wizard:

1. In the **Configuration** window click **Quick Start**. If you cannot see the **Quick Start** button, first click **My Project** in the **Project** window.



2. In the **Select Project Type** window click to select the type of calculation to perform. **Single point equilibrium**, **Property diagram**, **Phase diagram** or **Scheil solidification simulation**. Click **Next**.



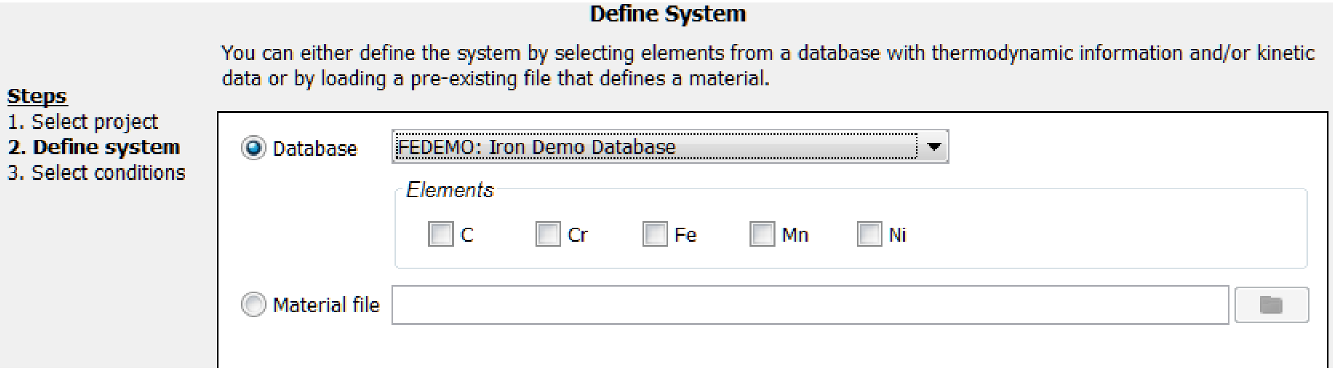
Select Project Type

Select the kind of calculation that you want to perform.

Steps
1. Select project
2. Define system
3. Select conditions

● Single point equilibrium
○ Property diagram
○ Phase diagram
○ Scheil solidification simulation

3. In the **Define Systems** window, choose an available **Database**.



Define System

You can either define the system by selecting elements from a database with thermodynamic information and/or kinetic data or by loading a pre-existing file that defines a material.

Steps
1. Select project
2. Define system
3. Select conditions

● Database: FEDEMO: Iron Demo Database

Elements

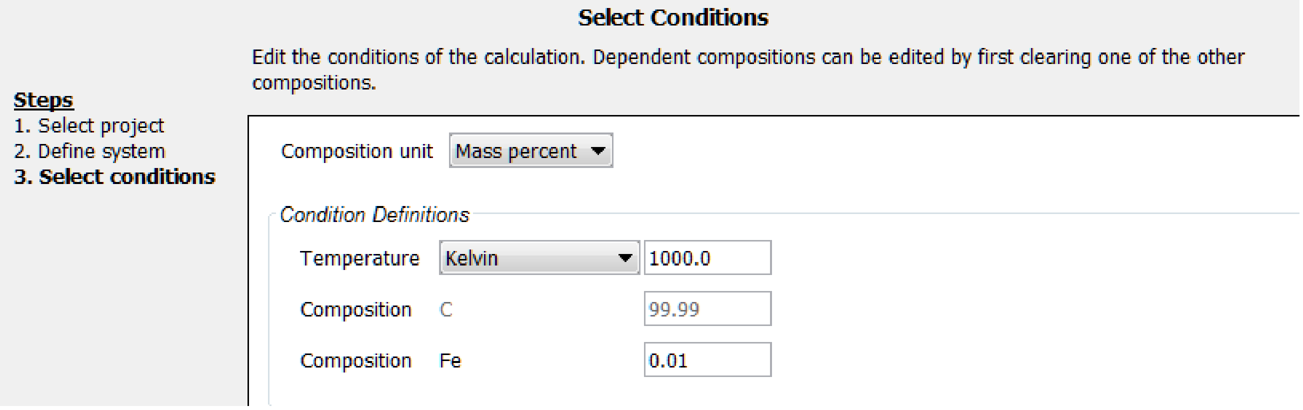
☐ C ☐ Cr ☐ Fe ☐ Mn ☐ Ni

○ Material file

4. Click to select **Elements** check boxes to include as system components. To add elements from an existing material file, click the **Material file** button to enter the file path to a material file or click the **Select Material File** button (to the right of the field) to navigate to a file on the computer.
5. Click **Next**.

The **Select Conditions** window has different options depending on the Project type and the elements selected.

In this example figure, using a **Single Point Equilibrium**, choose the **Composition unit** and under **Condition Definitions** specify the values of the state variables in the system.



Select Conditions

Edit the conditions of the calculation. Dependent compositions can be edited by first clearing one of the other compositions.

Steps
1. Select project
2. Define system
3. Select conditions

Composition unit: Mass percent

Condition Definitions

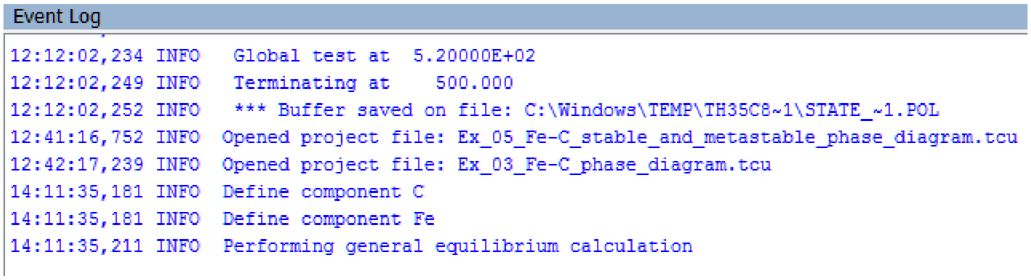
Temperature: Kelvin 1000.0
Composition C: 99.99
Composition Fe: 0.01

For a **Property diagram** or **Phase diagram**, specify the **Axis Definitions** of the stepping or mapping operation. Choose minimum and maximum values for the variable(s) (select **Linear – min no. of steps**, **Linear – max step size** or **Logarithmic –scale factors**) and whether it is **Normal** or **Separate phases**.

For a **Scheil solidification simulation**, and where applicable, select **Fast diffuser** to account for back-diffusion of any fast-diffusing elements.

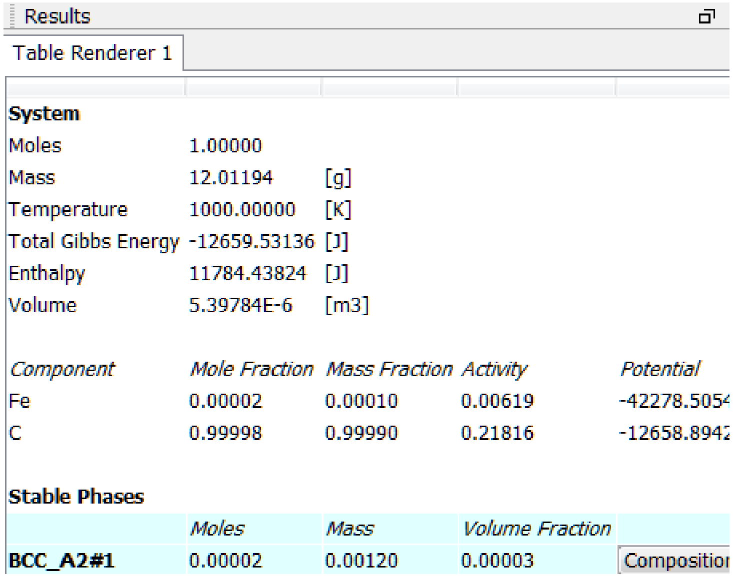
6. Click **Finish**.

7. Click to expand the **Event Log** window to see information about the progress of the calculation.



```
12:12:02,234 INFO   Global test at  5.20000E+02
12:12:02,249 INFO   Terminating at    500.000
12:12:02,252 INFO   *** Buffer saved on file: C:\Windows\TEMP\TH35C8~1\STATE_~1.POL
12:41:16,752 INFO  Opened project file: Ex_05_Fe-C_stable_and_metastable_phase_diagram.tcu
12:42:17,239 INFO  Opened project file: Ex_03_Fe-C_phase_diagram.tcu
14:11:35,181 INFO  Define component C
14:11:35,181 INFO  Define component Fe
14:11:35,211 INFO  Performing general equilibrium calculation
```

8. The diagram is plotted in a **Plot Renderer** tab in the **Results** window. If you have calculated a single-point equilibrium, then a **Table Renderer** tab shows information about the equilibrium.



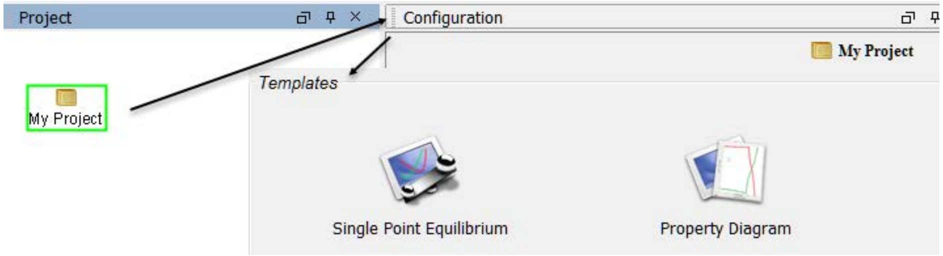
System				
Moles	1.00000			
Mass	12.01194	[g]		
Temperature	1000.00000	[K]		
Total Gibbs Energy	-12659.53136	[J]		
Enthalpy	11784.43824	[J]		
Volume	5.39784E-6	[m3]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Fe	0.00002	0.00010	0.00619	-42278.505
C	0.99998	0.99990	0.21816	-12658.894
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.00002	0.00120	0.00003	Compositio

9. To save the project, click **Save** on the main toolbar. To save a diagram or table, right-click the diagram or table and select **Save As**.

Creating a Project from a Template

Use a *Template* to create all the activities for a certain type of calculation. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window as in

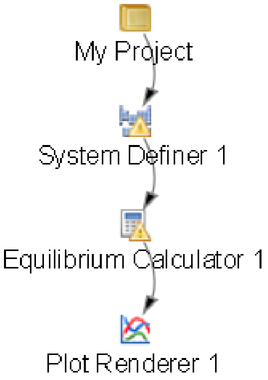
Configuration Window Templates



When you click a template, an activity tree is added to the Project window. You can then configure and perform the activities or the project.

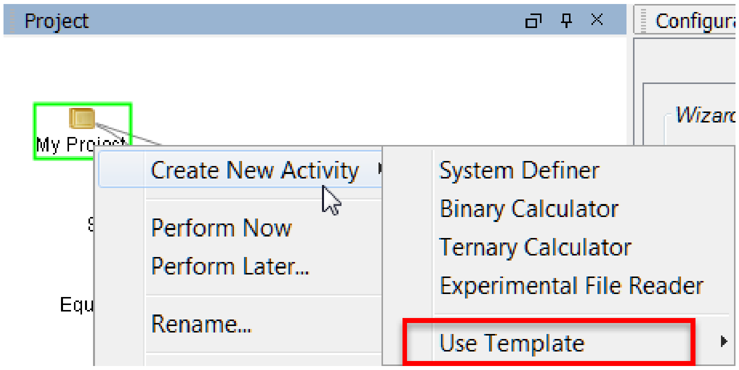
For example, if you click **Property Diagram**, a tree is added to the **My Project** node with **System Definer**, **Equilibrium Calculator** and **Plot Renderer** nodes.

Property Diagram Template



You can also select templates from the Project window. Right-click the **My Project** node and choose templates from the **Create New Activity → Use Template** submenu.

Use Template Submenu



Cloning Activities and Trees

As described in *Creating Activities and Successors* on page 30, you can clone a single activity or the selected activity and all the activities that come after it (successors). The predecessor of the selected activity also is the predecessor of the clone.

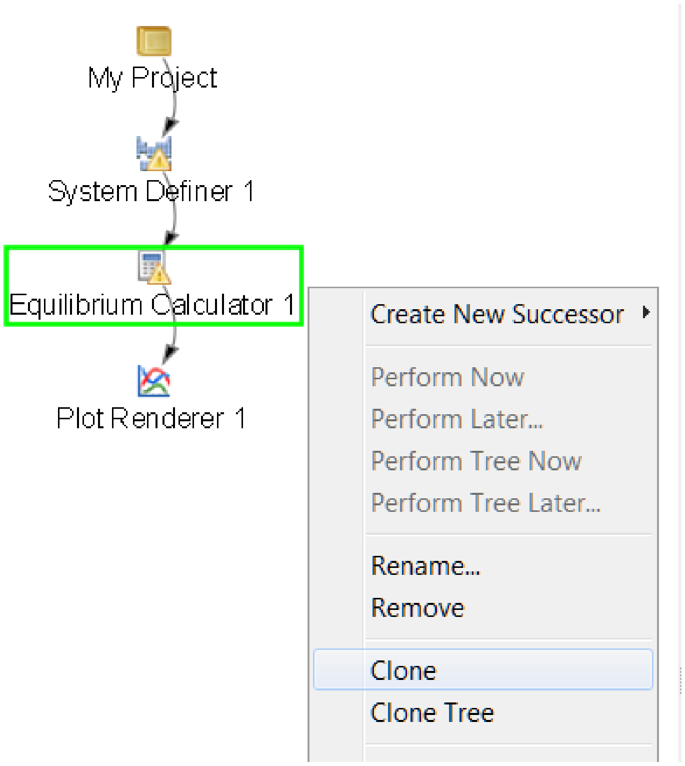
Cloned activities are configured exactly like the activities that they were cloned from, and any results of calculations or plots are also cloned. To clone a selected activity, right-click the activity and select **Clone**.

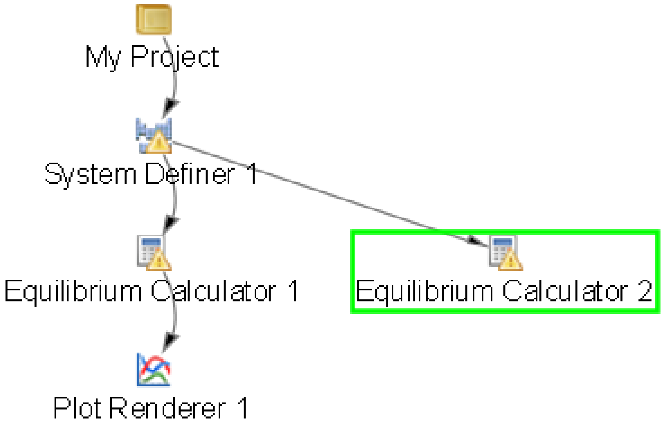
For example, if you clone the Equilibrium Calculator in this project the result is an **Equilibrium Calculator 2** created as a successor to **System Definer 1**.

The following applies to clones.

- The new Equilibrium Calculator has the same settings for conditions, functions and options as its Equilibrium Calculator 1 clone.
- If the Equilibrium Calculator is already performed, then the calculation results are cloned.
- If the activity is a Plot Renderer or a Table Renderer, then the plot or table is cloned.
- If you want to clone all the successor activities that follow a selected activity, then right-click and select **Clone Tree** instead.

Cloning an Equilibrium Calculator Activity Node





Equilibrium Calculator Clones and Successors

If you create an Equilibrium Calculator as a successor to another Equilibrium Calculator, then the successor inherits all the settings for conditions, functions and options from its predecessor. In this respect, it is similar to a clone.

The Equilibrium Calculator successor is different from a clone in that it does not inherit any calculated results and it is a successor to the Equilibrium Calculator instead of a successor to its predecessor.

The calculated result from an Equilibrium Calculator that is the predecessor to another Equilibrium Calculator is the starting value for the latter's calculation. The clone of an Equilibrium Calculator on the other hand, does not receive any data as input from the Equilibrium Calculator that it is cloned from.

Performing Projects, Trees and Activities

You can trigger the performance of an activity (also called a *job*) and all the activities below it in the same tree in either the **Project** or **Configuration** window. In the Project window you can also perform a single activity without performing its successors or perform the whole project (all the activity trees).

In the **Configuration** window, click **Perform Tree** to perform the currently selected activity and all the activities below it. If there are no activities below the selected activity, then the button says **Perform** instead.

All activities that must be completed as prerequisites are automatically performed first. For example, if you Perform Tree for a Plot Renderer, then the predecessors, Equilibrium Calculator and System Definer, are automatically performed before the Plot Renderer.

In the Project window, you can do any of the following:

- *Perform an activity*: Right-click the activity and select **Perform Now**, or **Perform Later** and schedule a time to perform the activity.
- *Perform an activity and all activities below it in the tree*: Right-click any node in the tree and select **Perform Tree Now**. Or select **Perform Tree Later** and schedule a time for all activities in the tree to be performed.
- *Perform a project*: Right-click **My Project** and select **Perform Now** or **Perform Later** and schedule a time to perform all project activities in the tree.

If there is an error during the performance of an activity, icons display status markers, which are described in *Node Status Markers* on page 41.

Using the Scheduler

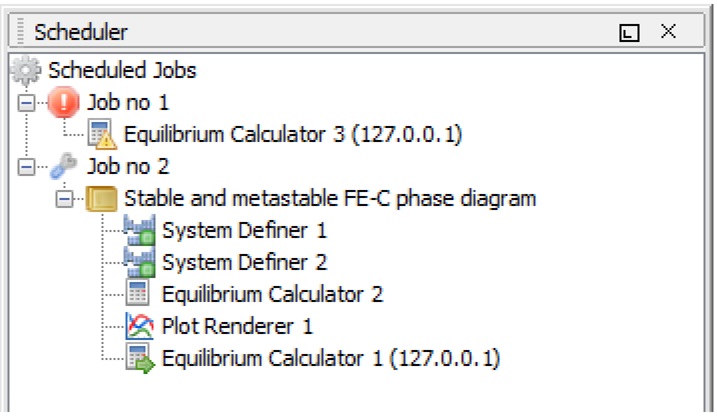
The **Scheduler** window has activity information about current or scheduled jobs. A *job* is any activity you have selected to be performed. The Scheduler also indicates if there is an error during a job and when a job has stopped. If you have set an activity, tree or project to be performed at a later time then this is also listed.

The following applies to jobs.

- Whenever you trigger the performance of a whole project, tree or individual activity, all the activities to be performed are shown under a job heading.
- When all the activities belonging to a job are completed the job and its activities disappear from the Scheduler window.
- If there is an error during the performance of an activity, icons for that job and activity remain in the Scheduler window until removed.

Also see *Node Status Markers* on page 41.

Scheduled Jobs Example



Scheduler

Scheduled Jobs
- Job no 1
  - Equilibrium Calculator 3 (127.0.0.1)
- Job no 2
  - Stable and metastable FE-C phase diagram
    - System Definer 1
    - System Definer 2
    - Equilibrium Calculator 2
    - Plot Renderer 1
    - Equilibrium Calculator 1 (127.0.0.1)

Managing the Schedule

In the Scheduler window, you can cancel scheduled jobs, remove errors and show information about errors.

- To cancel all jobs, right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Cancel All Jobs**.
- To remove (clear) all failed activities and jobs, right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Clear All Errors**.
- To cancel a specific job, right-click the job label (for example, **Job no 1**) and select **Cancel Job**.
- To remove (clear) a specific failed job, right-click the job label (for example, **Job no 1**) and select **Cancel Job**.
- To open a window with error details, right-click the label for the failed job (for example, **Job no 1**), and select **Show Error Log**.

The Event Log

The **Event Log** window is closed by default. Click the **Event Log** window once to expand it or select it from the **Window→Event Log** menu. Double-clicking the window maximizes the window.

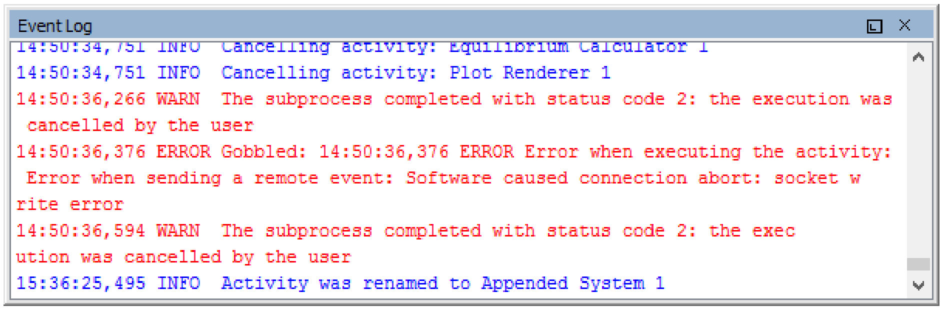
Information about what Thermo-Calc is processing or doing is in blue text and error or warning messages are in red text.

To specify the level of detail in the Event Log window, from the main menu select **Tools →Options**. In the **General** tab set the **Log level** slide bar to anything between **Debug** (most detailed) and **Error** (least detailed).

Also see *Changing Global Settings* on page 189.

Event Log Window Example

The example shows information, warnings and errors.



```
14:50:34,751 INFO  Cancelling activity: Equilibrium Calculator 1
14:50:34,751 INFO  Cancelling activity: Plot Renderer 1
14:50:36,266 WARN  The subprocess completed with status code 2: the execution was
 cancelled by the user
14:50:36,376 ERROR Gobbled: 14:50:36,376 ERROR Error when executing the activity:
 Error when sending a remote event: Software caused connection abort: socket w
rite error
14:50:36,594 WARN  The subprocess completed with status code 2: the exec
ution was cancelled by the user
15:36:25,495 INFO  Activity was renamed to Appended System 1
```

Graphical Mode Activities

These topics describe the activity types and has instructions for procedures tied to specific activities.

In this section:

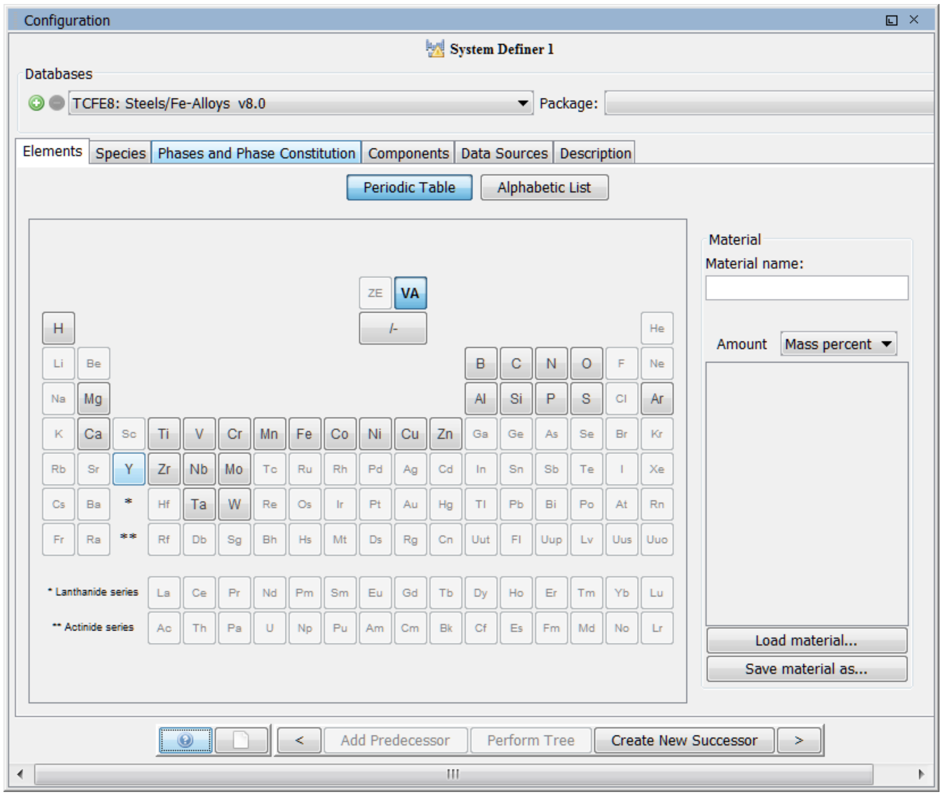
System Definer

In a System Definer activity, you select the database to use to retrieve thermodynamic data and define which elements the system has as components. You can also select which species to include as well as change the reference temperature and pressure for your components.

Also see *Creating Activities and Successors* on page 30 for a list of possible successors and predecessors for this activity.

The System Definer Settings

Configuration Window

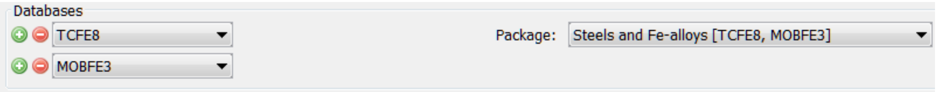


Databases: TCFE8: Steels/Fe-Alloys v8.0

Package:

Amount: Mass percent

Choose Database(s) or a Database Package



Databases: TCFE8, MOBFE3

Package: Steels and Fe-alloys [TCFE8, MOBFE3]

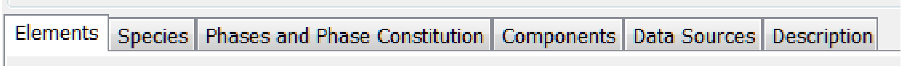
At the top of the **Configuration** window you can choose to add one or more databases by clicking the **Add a database** button. You can also choose a predefined or custom database package from the **Package** list. Depending on your license, there are predefined database packages available to select.

You can also click **Remove this database** button as required.

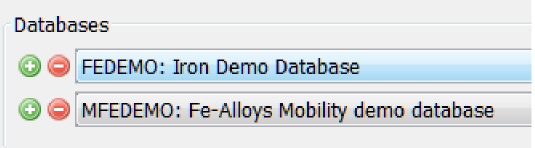
Also see *Global Settings: System Definition (System Definer)* on page 192 to learn how to create a database package.

If you have chosen a database package and then remove or change a database, a message displays *Selected databases and selected package may differ*. This means that the original package you selected, which added preset databases, does not match the databases you are using for the project. For information about how to clear the message, see *Global Settings: System Definition (System Definer)* on page 192.

There are several settings tabs available for the System Definer activity.



The following example uses the FEDEMO and MFEDEMO databases and Example 12 available with the *Graphical Mode Example Collection* on page 9.


Databases

FEDEMO: Iron Demo Database

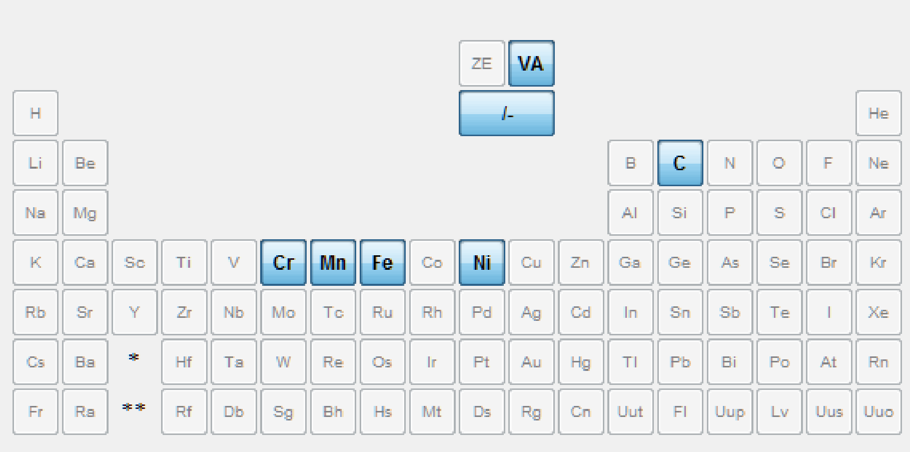
MFEDEMO: Fe-Alloys Mobility demo database

Elements

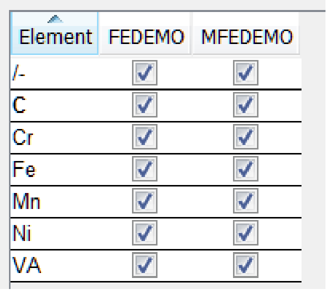
On the **Elements** tab, and based on the databases or database package selected, you can select and review elements using a **Periodic Table** or **Alphabetic List** format. Unavailable elements are greyed out on the Periodic Table view.

Periodic Table

In this example, using the demonstration databases FEDEMO and MFEDEMO, there are only a select number of elements to choose from.



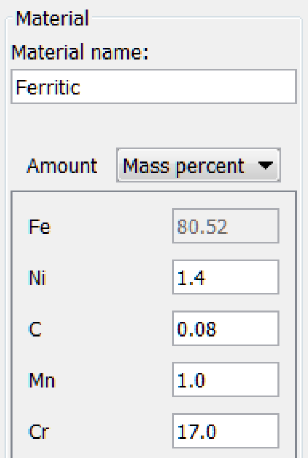
Alphabetic List



Element	FEDEMO	MFEDEMO
/-	☑	☑
C	☑	☑
Cr	☑	☑
Fe	☑	☑
Mn	☑	☑
Ni	☑	☑
VA	☑	☑

Material Composition

On the **Periodic Table** page, you can also define the material composition:



Material

Material name: Ferritic

Amount: Mass percent

Fe	80.52
Ni	1.4
C	0.08
Mn	1.0
Cr	17.0

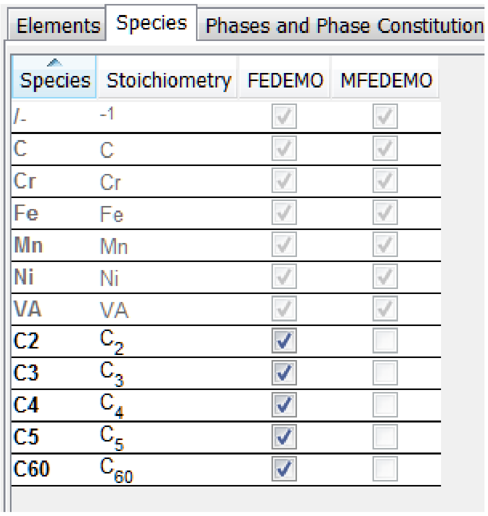
At the bottom of the window, click **Load material** to open a material file. Click **Save material as** to save the material you defined, for example **Ferritic**.

Also see *Global Settings: System Definition (System Definer)* on page 192 to learn how to create your own database packages.

If you Load a material file and then change the composition, a message displays *The composition has changed*. This means that the original values/composition does not match the values you are using for the project. The message is cleared by either reloading the material file or editing the composition field to the original value.

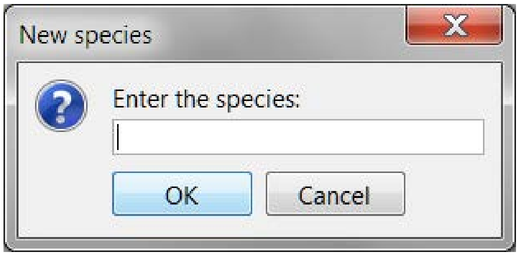
Species

On the **Species** tab for each database you can select and edit the **Species**.



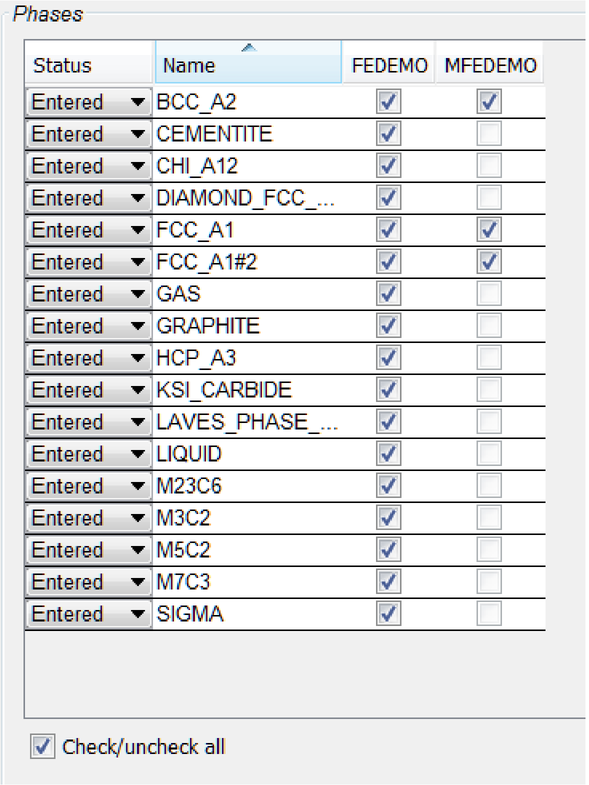
Species	Stoichiometry	FEDEMO	MFEDEMO
/-	-1	☑	☑
C	C	☑	☑
Cr	Cr	☑	☑
Fe	Fe	☑	☑
Mn	Mn	☑	☑
Ni	Ni	☑	☑
VA	VA	☑	☑
C2	C_2	☑	☐
C3	C_3	☑	☐
C4	C_4	☑	☐
C5	C_5	☑	☐
C60	C_{60}	☑	☐

At the bottom of the window, click **Add new species** and enter the name of species in the field.



.

Phases and Phase Constitution



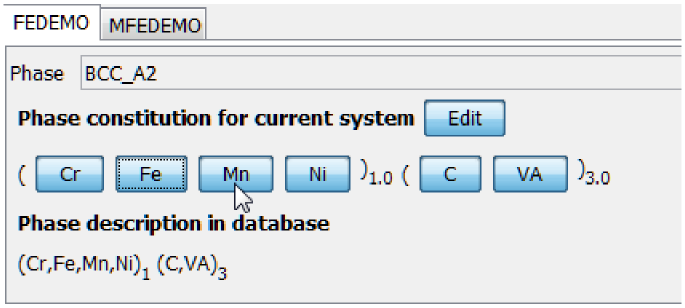
Phases

Status	Name	FEDEMO	MFEDEMO
Entered	BCC_A2	☑	☑
Entered	CEMENTITE	☑	☐
Entered	CHI_A12	☑	☐
Entered	DIAMOND_FCC_...	☑	☐
Entered	FCC_A1	☑	☑
Entered	FCC_A1#2	☑	☑
Entered	GAS	☑	☐
Entered	GRAPHITE	☑	☐
Entered	HCP_A3	☑	☐
Entered	KSI_CARBIDE	☑	☐
Entered	LAVES_PHASE_...	☑	☐
Entered	LIQUID	☑	☐
Entered	M23C6	☑	☐
Entered	M3C2	☑	☐
Entered	M5C2	☑	☐
Entered	M7C3	☑	☐
Entered	SIGMA	☑	☐

☑ Check/uncheck all

At the top of the **Phases and Phase Constitution** tab for each database, you can review and edit the **Status** (**Entered** or **Dormant**) for the selected**Phases**. Select the **Check/uncheck all** check box to toggle between the options.

To review the **Phase constitution** for a specific phase, click it in the **Phase** list (for example **BCC_A2**) and its details are displayed at the bottom of the window. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.



Phase: BCC_A2

Phase constitution for current system

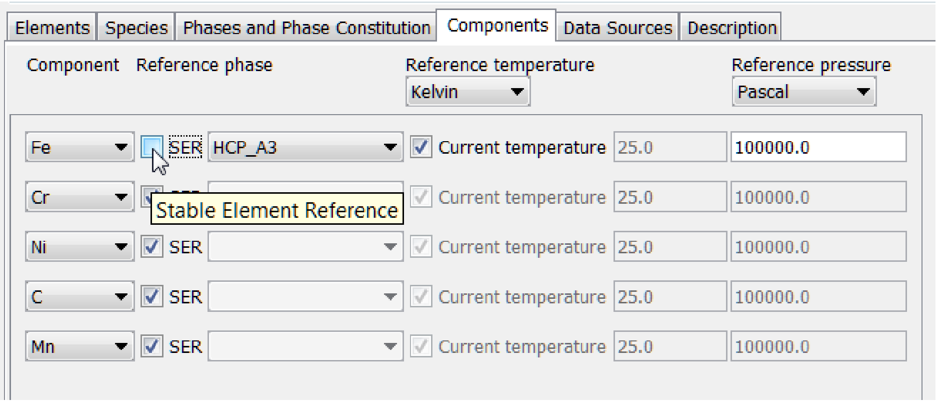
(Cr Fe Mn Ni $)_{1.0}$ (C VA $)_{3.0}$

Phase description in database

$(Cr,Fe,Mn,Ni)_1\ (C,VA)_3$

Components

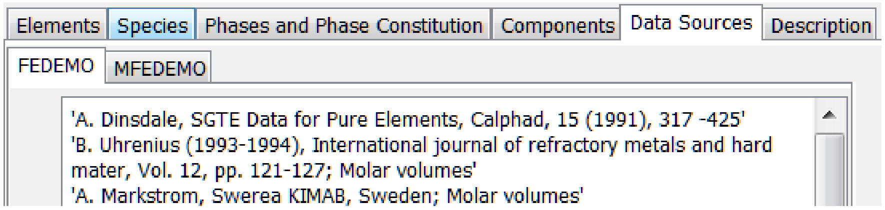
The **Components** tab is where you can review and edit the **Component**, **Reference phase**, **Reference temperature**, and **Reference pressure**. Click to toggle the **SER** (Stable Element Reference) check box on and off. Then choose a **Reference phase** from the list and edit accordingly.



Component		Reference phase		Reference temperature (Kelvin)	Reference pressure (Pascal)
Fe	☐ SER	HCP_A3	☑ Current temperature	25.0	100000.0
Cr	☑ SER		☑ Current temperature	25.0	100000.0
Ni	☑ SER		☑ Current temperature	25.0	100000.0
C	☑ SER		☑ Current temperature	25.0	100000.0
Mn	☑ SER		☑ Current temperature	25.0	100000.0

Data Sources

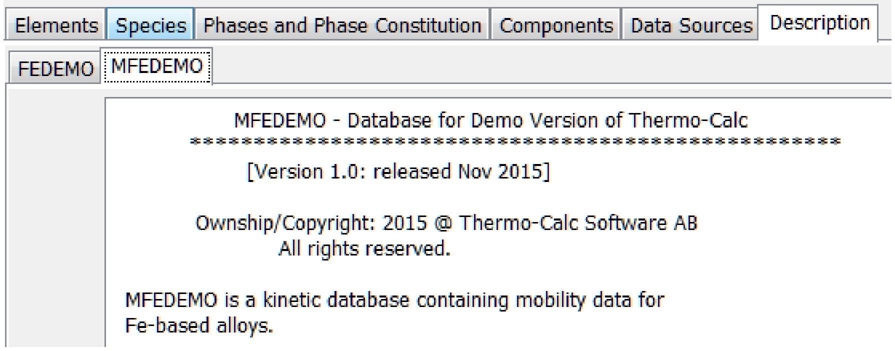
Data sources are not available until the activity has been performed. Click **Perform Tree** to display available data sources.



'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
'B. Uhrenius (1993-1994), International journal of refractory metals and hard mater, Vol. 12, pp. 121-127; Molar volumes'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'

Description

The **Description** tab displays a description of the selected database(s). In this example, **MFEDEMO**.



MFEDEMO - Database for Demo Version of Thermo-Calc
****
[Version 1.0: released Nov 2015]

Ownship/Copyright: 2015 @ Thermo-Calc Software AB
All rights reserved.

MFEDEMO is a kinetic database containing mobility data for Fe-based alloys.

Creating a System Definer Activity

This topic describes how to define a system; specifically how to select one or more databases and define the elements in the system.

To change the default database or create a database package, see *Global Settings: System Definition (System Definer)* on page 192.

Also see *About the Database Files* on page 186.

1. Right-click **My Project** and from the menu select **Create New Activity→ System Definer** .
2. In the **Project** window, click the *System Definer* on page 55 activity node.
3. In the **Configuration** window, from the **Databases** menu choose **Database(s)** or a **Database Package**.

   Options are to:

- Select **<User database>**to define your own.
- You can choose to add one or more databases by clicking the **Add a database** ⊕ button.
- From the **Package** list, choose a predefined database package to add multiple databases at a time. Depending on your license, there are predefined database packages available to select.

4. Select the **Elements** tab to choose the elements in the **Periodic Table** or use the **Alphabetic List** to choose elements for the system.
5. As required click the tabs to make edits: **Species**, **Phases and Phase Constitution**, and **Components**. The **Data Sources** and **Description** tabs provide information based on the database.
6. Click **Perform** to start the System Definer activity immediately and retrieve thermodynamic data about the system. Click the **Event Log** window to watch the progress of the job.

Property Model Calculator

A Property Model Calculator allows you to predict and optimize material properties. A set of general models is available to use: a *Phase Transition Model* on page 69, *Driving Force Model* on page 70, *Interfacial Energy Model* on page 71, *Coarsening Model* on page 71, and an *Equilibrium Model* on page 73.

You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot. The **Configuration** window for a Property Model Calculator using the *Phase transition* model is shown and described in *Defining the Property Model Calculator* on page 65.

Property Model Calculator Workflow

When a project is first being designed, it is recommended you test it by first performing a **Single** calculation type. This verifies that the configuration of the model is valid, otherwise you will get a *Not a Number* result in *Event Log Window* on page 118 window indicating the calculation did not work correctly.

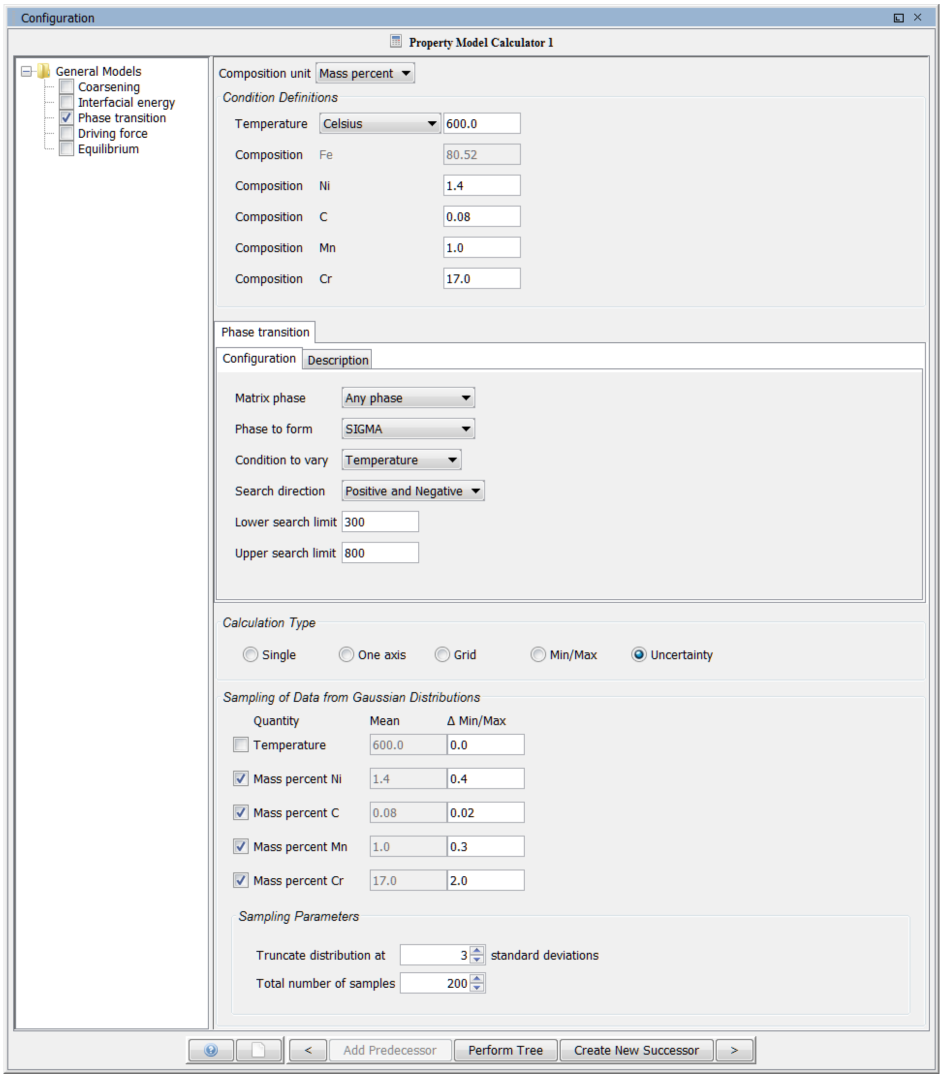
Once the Single calculation type performs successfully, you can experiment with other calculation types such as **Grid**, **Min/Max** or **Uncertainty**. Best practice for both Grid and Uncertainty is to start with a small number of steps (Grid) or samples (Uncertainty) to confirm that it works before increasing the number of steps or samples.

In general, the workflow for the different models will differ. A recommended start point is to do a Property Diagram calculation to determine what phases you get and where the transitions are before setting up the Property Model Calculator. You can create a Property Diagram using the Quick Start wizard or a template.

Also see *The Quick Start Wizard* on page 44 and *Creating a Project from a Template* on page 47.

For examples using the Property Model Calculator, see examples 10, 11, and 12 in *Graphical Mode Example Collection* on page 9.

Configuration Window



Composition unit: Mass percent

Condition Definitions

Temperature: Celsius 600.0
Composition Fe 80.52
Composition Ni 1.4
Composition C 0.08
Composition Mn 1.0
Composition Cr 17.0

Phase transition – Configuration | Description

Matrix phase: Any phase
Phase to form: SIGMA
Condition to vary: Temperature
Search direction: Positive and Negative
Lower search limit: 300
Upper search limit: 800

Calculation Type

○ Single ○ One axis ○ Grid ○ Min/Max ● Uncertainty

Sampling of Data from Gaussian Distributions

Quantity	Mean	Δ Min/Max
☐ Temperature	600.0	0.0
☑ Mass percent Ni	1.4	0.4
☑ Mass percent C	0.08	0.02
☑ Mass percent Mn	1.0	0.3
☑ Mass percent Cr	17.0	2.0

Sampling Parameters

Truncate distribution at 3 standard deviations
Total number of samples 200

Configuration Settings

Setting/Button	Description
Composition unit	Choose a unit: **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**
Condition Definitions	Choose a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and then enter a value for the **Temperature** and **Composition**. The values entered in Condition Definitions are used as the start values for the different calculation types.
Calculation Type	Choose a calculation type: **Single** (no axes), **One axis**, **Grid**, **Min/Max** or **Uncertainty**. Select **Single** to calculate a single point.

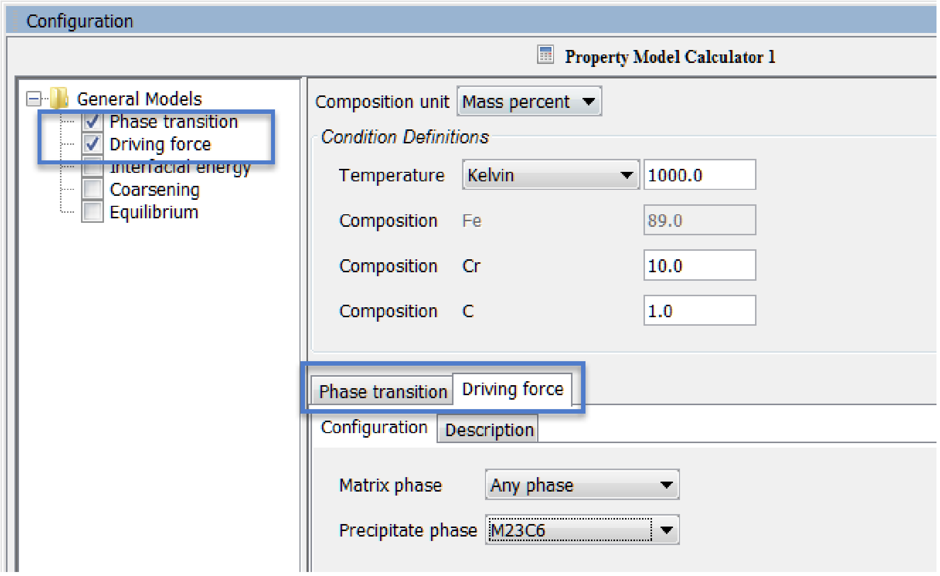
Setting/Button	Description
	Select **One axis** to vary a quantity on the X-axis. Select a **Grid** to evaluate two axis variables of the selected quantities in the specified range and number of steps. The **Min/Max** calculation evaluates the property model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under Condition Definitions for the respective quantity. The total minimum and maximum of the model(s) results are shown in the Event log. The **Uncertainty** calculation evaluates the property model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under Condition Definitions for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.
Single calculation	For the **Single** calculation type no further settings are required. The results from this calculation are displayed in the **Event Log**.
Axis Definition	For **One axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max** and **Number of steps**.
Grid Definitions	For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max** and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected models are evaluated.
Min/Max Definitions	For the **Min/Max** calculation type, click to select the applicable check boxes under **Quantity to enable or disable an axis**. The **Mean** field is as defined under Condition Definitions for the respective quantity. Enter numerical values in the Δ **Min/Max** fields to evaluate the change to the quantity. The highest and lowest value of each selected model results are shown in the Event log.
Sampling of Data from Gaussian Distributions	For the **Uncertainty** calculation type, click to select the applicable check boxes under **Quantity to vary this quantity**. The **Mean** field is for the distribution function as defined under Condition Definitions for the respective quantity. ΔMin/Max is the 95% confidence interval.
Sampling Parameters	For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

Also see *About the Uncertainty Calculations* on the next page for more detail.

Defining the Property Model Calculator

1. From the left side of the Configuration window, click to select one or more of the check boxes under the **General Models** folder.

   A tab with the same name as the property model opens in the right side of the window under *Condition Definitions*. When you select more than one model, a matching tab is added in the same order that the check box is selected.



☑ Phase transition
☑ Driving force
☐ Interfacial energy
☐ Coarsening
☐ Equilibrium

Composition unit: Mass percent

Condition Definitions

Temperature: Kelvin 1000.0
Composition: Fe 89.0
Composition: Cr 10.0
Composition: C 1.0

Matrix phase: Any phase
Precipitate phase: M23C6

2. Enter the settings described in the following table for the *Condition Definitions* and for each *Calculation Type* (Single, Grid, Min/Max, and Uncertainty). For each model on the **Configuration** tab, select or enter settings as required. Click the **Description** tab for more information about the model and refer to the individual sections for details.

   - *Phase Transition Model* on page 69
   - *Driving Force Model* on page 70
   - *Interfacial Energy Model* on page 71
   - *Coarsening Model* on page 71
   - *Equilibrium Model* on page 73

About the Uncertainty Calculations

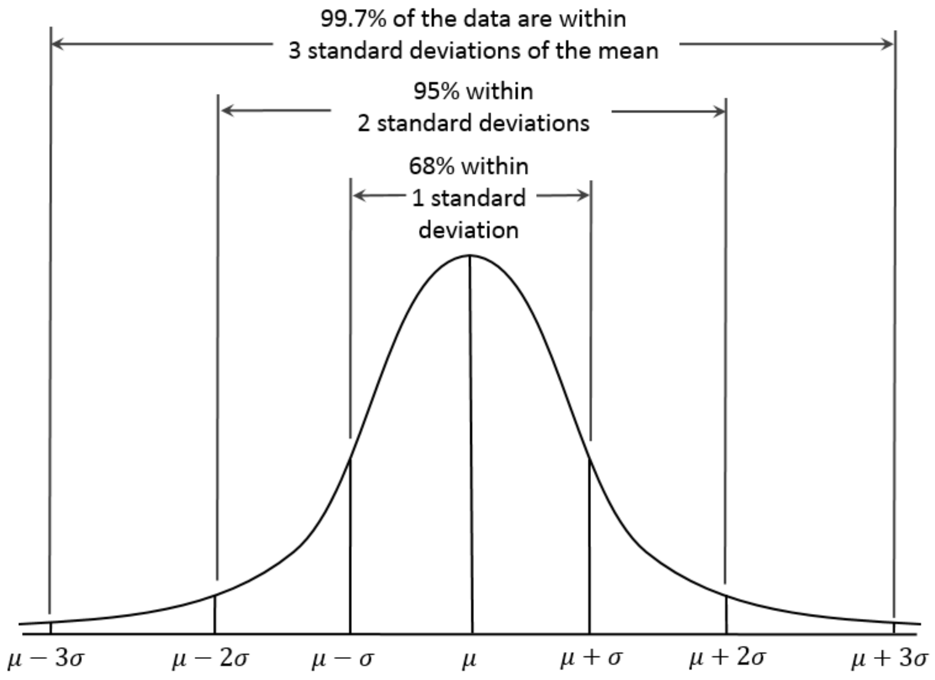
The following example uses the *Phase Transition Model* on page 69 and an **Uncertainty Calculation Type** to describe how the sampling of data is performed. The example (which is example 10 in *Graphical Mode Example Collection* on page 9) predicts the transition temperature to the unwanted brittle Sigma phase and shows how the temperature is influenced by changes to a steel alloy's composition.

The **Uncertainty** calculation in Thermo-Calc uses the values (the mean) entered for quantities in the Condition Definitions section as the starting point to estimate, within a certain probability, the true variation of the quantity.

An example of a Gaussian distribution is shown The *mean* is at the peak of the curve (labelled μ). The *standard deviation* (σ) is a plus and minus range, ±1σ, ±2σ or ±3σ, of the variance from the mean.

Gaussian Distribution, the 3-Sigma Rule

Image by Dan Kernler, https://en.wikipedia.org/wiki/Normal_distribution#/media/File:Empirical_Rule.PNG

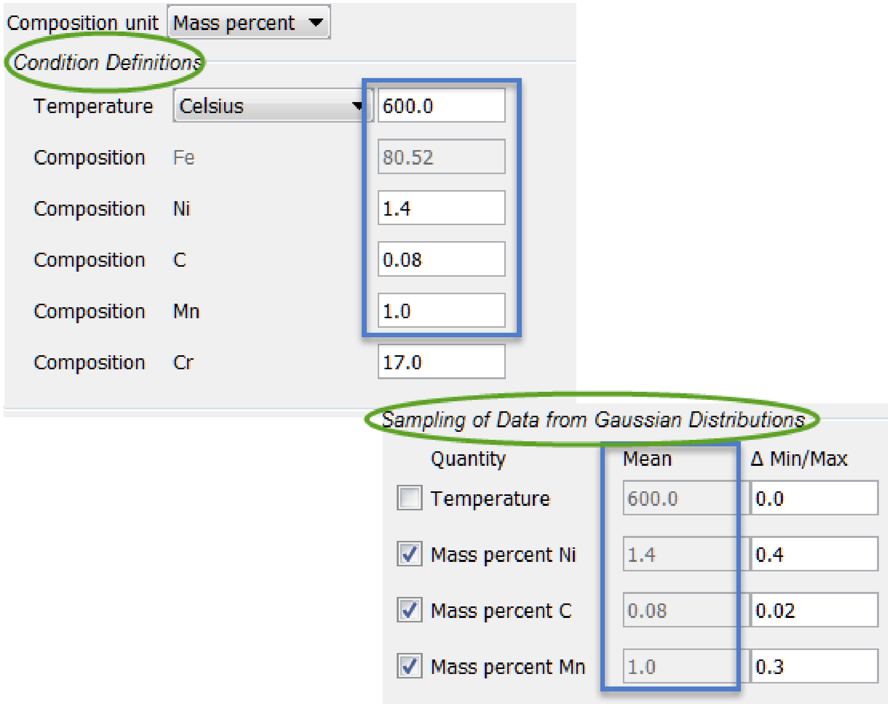


As long as the number of events (the sample size) is very large, then the Gaussian distribution function can be used to describe physical events. A Gaussian distribution is assumed to describe how each quantity varies in an uncertainty calculation.

In Thermo-Calc, the mean of the quantity's distribution is defined in the *Condition Definitions* section. The **Mean** is then used in the *Sampling of Data from Gaussian Distributions* section as the starting point for how much you want to deviate from this value.

Condition Definitions and Sampling Settings

The mean defined in Condition Definitions is used during the sampling.



Composition unit: Mass percent

Condition Definitions

Temperature	Celsius	600.0
Composition	Fe	80.52
Composition	Ni	1.4
Composition	C	0.08
Composition	Mn	1.0
Composition	Cr	17.0

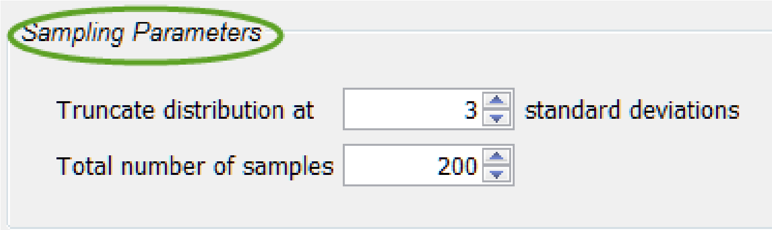
Sampling of Data from Gaussian Distributions

Quantity	Mean	Δ Min/Max
☐ Temperature	600.0	0.0
☑ Mass percent Ni	1.4	0.4
☑ Mass percent C	0.08	0.02
☑ Mass percent Mn	1.0	0.3

The values entered in the **Δ Min/Max** fields are the resulting width of the distribution corresponding to the 95% confidence interval (approximately $\mu \pm 2\sigma$) shown in *Gaussian distribution, the 3-sigma rule*.This confidence interval means that approximately 95% of the sampled values will fall within these limits.

The default value for truncating the distribution is set at **3 standard deviations** in the *Sampling Parameters* section. This is also where you set the **Total number of samples**. The default is 200. In order to maintain a Gaussian distribution for the varied quantities, this number should not be too low.

Sampling Parameter Settings



Sampling Parameters

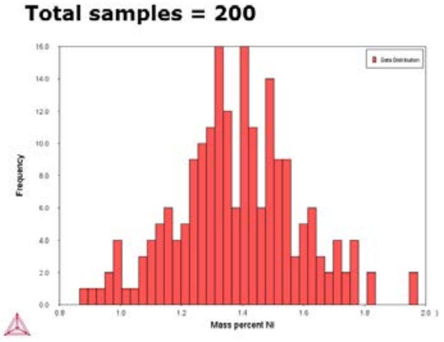
Truncate distribution at: 3 standard deviations

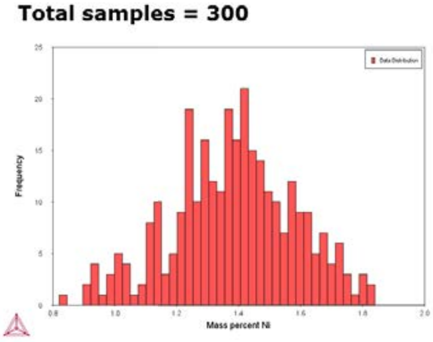
Total number of samples: 200

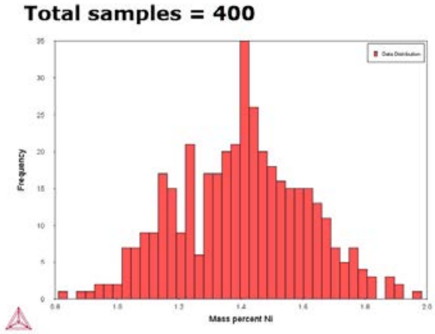
You can experiment by varying the conditions and the number of samples to see the distribution results smooth out as is to be expected based on the Central Limit Theorem. For example, on the **Plot Renderer** the variable is set to measure the **Composition** of **Ni**. The initial sample size uses the default, 200, and then, as in the example below where the sample size is increased to 300, 400, 600, 800, and 1000 to show how the plot follows the Gauss distribution.

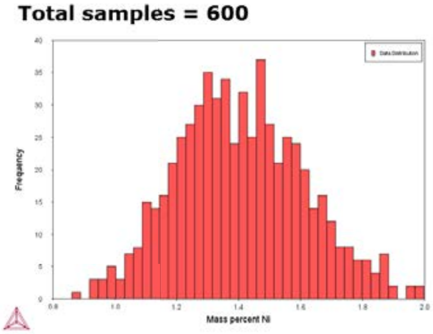
Histogram Plot

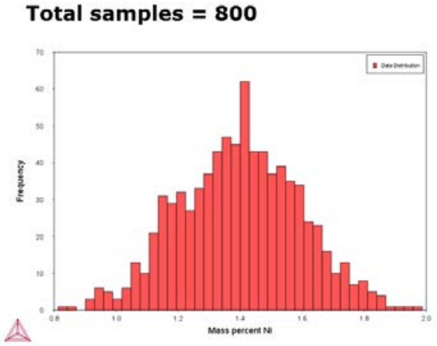
This is a series of histogram plots of the uncertainty calculations sampling data from Gaussian distributions. It compares the Ni composition where the total sample size is increased to show how the model follows the Gauss distribution.

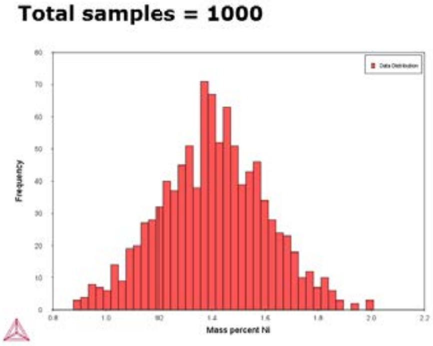

Total samples = 200


Total samples = 300


Total samples = 400

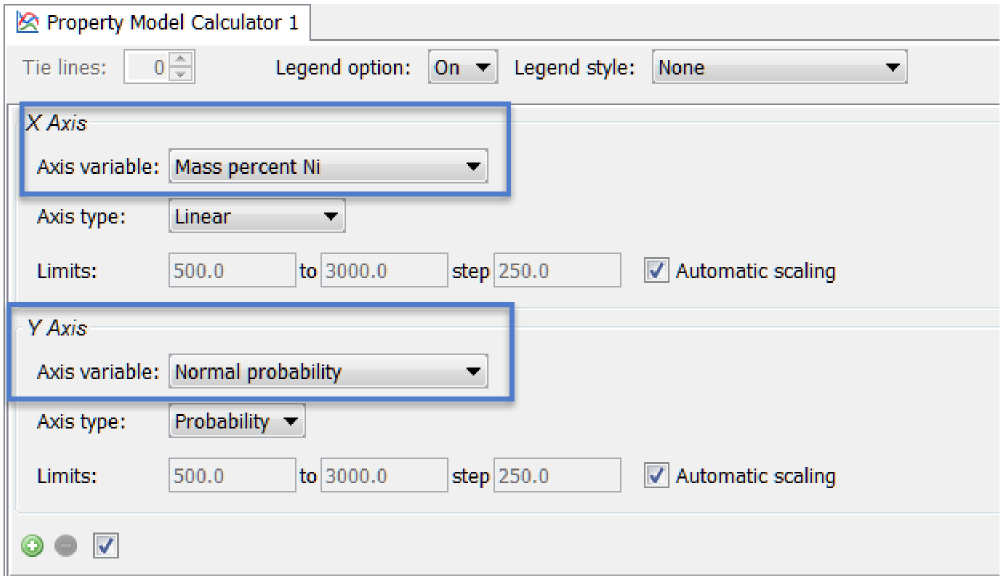

Total samples = 600


Total samples = 800


Total samples = 1000

Normal Probability Plot

You can also plot the results as a Normal probability. Continuing with this example, on the Property Model Calculator Configuration window the X-Axis variable is plotted as Composition and the Y-Axis variable is plotted as the Normal probability.



Property Model Calculator 1

Tie lines: 0

Legend option: On

Legend style: None

X Axis

Axis variable: Mass percent Ni

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

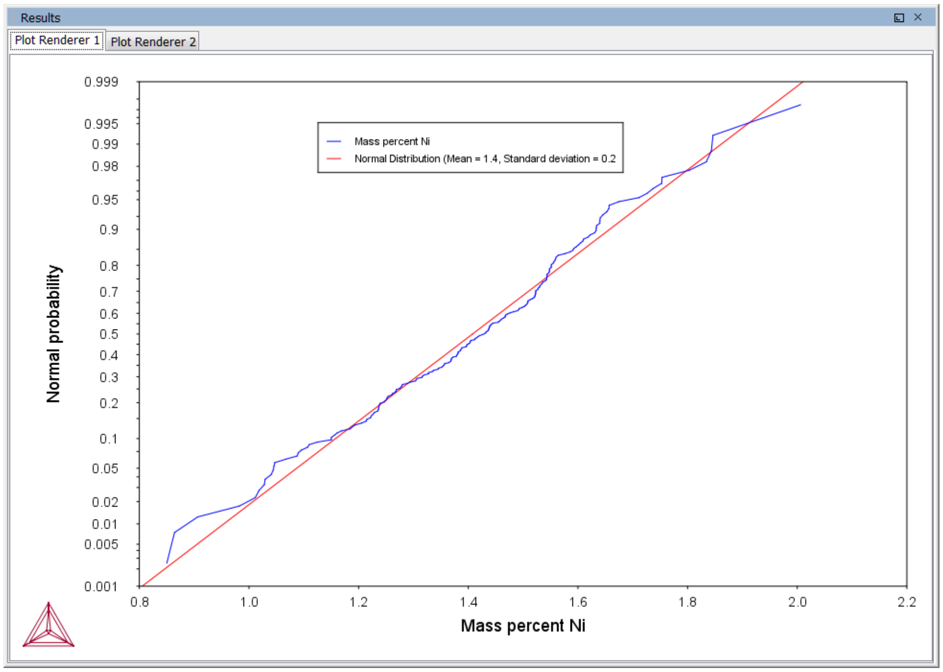
Y Axis

Axis variable: Normal probability

Axis type: Probability

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

This is a normal probability plot example of the uncertainty calculations sampling data from Gaussian distributions. It compares the Ni composition where the total sample size is 200. The sampled data (blue line) closely follows the ideal normal distribution (red line). Deviations are naturally larger at the tails (≈1%Ni and ≈2%Ni) since the number of samples are fewer there compared to the center of the distribution.



Phase Transition Model

By varying set conditions, the **Phase Transition** model calculates the point when a new phase may form. The model is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the varied condition.

For an example of a phase transition model, see example 10 in *Graphical Mode Example Collection* on page 9.

Define the:

- **Matrix phase** - The single phase region to start in. Select 'Any phase' to use the phases that take part of the initial equilibrium or choose a specific phase.
- **Phase to form** - For the new phase to be formed, select 'Any phase' or choose a specific phase.
- **Condition to vary** – Choose whether to vary a composition or temperature condition when calculating the phase transition.
- **Search direction** - For the composition or temperature condition being varied, choose the Search direction to be in a **Positive**, **Negative**, or **Positive and Negative** direction.
- **Upper search limit** and **Lower search limit** - These values also relate to the search direction, where an estimated change to the released condition implies where a new phase is expected.

  The start value (given in Condition Definitions) and phase transition point need to be within these limits, otherwise the model returns *Not a Number* as result. For example, a start temperature is 1100 K then the limits need to be outside these, e.g. 500-1500.

Driving Force Model

The **Driving Force** model calculates the thermodynamic driving force for a phase.

- **Matrix phase**: Choose a **Matrix phase**, the single phase region to start in. Select 'Any phase' to use the phases that take part of the initial equilibrium or choose a specific phase.
- **Precipitate phase**: Choose a **Precipitate phase** to calculate its driving force.

  The calculation result is the driving force divided by RT.

For an example of a driving force model, see example 12 in *Graphical Mode Example Collection* on page 9.

Interfacial Energy Model

Use the **Interfacial Energy** model to estimate the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database. The approximation model is based on Becker's bond energy approach and is also available in Precipitation Module (TC-PRISMA). In the actual calculation, the coefficients taken distinguish between only bcc and fcc structure for the (110) and (111) lattice plane, respectively.

For other planes and/or other phases, the estimate is approximate. In most situations, it is recommended to perform calibrations against some experimental data because the interfacial energy is dependent on so many factors that are ignored in the estimation, for example entropy, incoherency, orientation, and curvature, etc. Uncertainty factors must also be considered as thermodynamic data in CALPHAD databases are not always accurate.

Select the **Matrix phase** and **Precipitate phase** to return the interfacial energy [J/m^2].

For an example of an interfacial energy model, see example 11 in *Graphical Mode Example Collection* on page 9.

Estimation of Coherent Interfacial Energy

Interfacial energy is an important parameter used in precipitation simulations to calculate the rates of nucleation, growth/dissolution, and coarsening. The value of interfacial energy can vary dramatically (usually between 0.01 to 2.0 J/m^2).

The extended Becker’s model functions to estimate coherent interfacial energy by using thermodynamic data from existing CALPHAD thermodynamic databases:

$$\sigma_c = \frac{n_s z_s}{N_A z_l} \Delta E_s$$

where σ_c is the coherent interfacial energy, n_s is the number of atoms per unit area at the interface, z_s is the number of cross bonds per atom at the interface, z_l is the coordination number of an atom within the bulk crystal lattice, and ΔE_s is the energy of solution in a multicomponent system involving the two phases being considered. (Reference[1]).

Coarsening Model

The **Coarsening** model calculates the coarsening rate coefficient K (m^3/s) of a spherical precipitate phase in a matrix phase.

- **Matrix phase**: Choose the **Matrix phase**.
- **Precipitate phase**: Choose a **Precipitate phase** to calculate its coarsening rate.

---

[1] Becker, R., Die Keimbildung bei der Ausscheidung in metallischen Mischkristallen, Ann. Phys. 424, 128–140 (1938).

Returns the coarsening rate coefficient [m^3/s] for the precipitate phase and the interfacial energy [J/m^2] between matrix and the precipitate phase.

This model requires that the thermodynamic and kinetic databases used include descriptions of molar volume of the matrix and precipitates as well as mobilities for the matrix phase.

For an example of a coarsening model, see example 11 in *Graphical Mode Example Collection* on page 9.

Particle Coarsening

In the coarsening regime where the driving force is capillarity, the change of mean particle radius evolves according to the equation:

$$\bar{r}^3 - \bar{r}_0^3 = Kt$$

Following Morral and Purdy, the rate constant of precipitating β phase in a multicomponent α phase is

$$K = \frac{8\sigma V_m^\beta}{9}\left[\left[c_i^\beta - c_i^\alpha\right]^T [M]^{-1}\left[c_k^\beta - c_k^\alpha\right]\right]^{-1} K = \frac{8\sigma V_m^\beta}{9}\left[\left[c_i^\beta - c_i^\alpha\right]^T [M]^{-1}\left[c_k^\beta - c_k^\alpha\right]\right]^{-1}$$

The mobility matrix M is not the same as the mobilites that can be obtained directly from the Diffusion Module (DICTRA). The M matrix instead corresponds to the L’’ matrix as defined by Andersson and Ågren.

Using the u-fractions that is defined as

$$u_k = \frac{x_k}{\sum_{j \in S} x_j}$$

where the summation only is performed over the substitutional elements give the final equation for the coarsening rate coefficient.

$$K = \frac{8\sigma V_m^\beta}{9}\left[\left[u_i^\beta - u_i^\alpha\right]^T \left[L''^{\alpha}_{jk}\right]^{-1}\left[u_k^\beta - u_k^\alpha\right]\right]^{-1} K = \frac{8\sigma V_m^\beta}{9}\left[\left[u_i^\beta - u_i^\alpha\right]^T \left[L''^{\alpha}_{jk}\right]^{-1}\left[u_k^\beta - u_k^\alpha\right]\right]^{-1}$$

The interfacial energy σ is calculated using the extended Becker’s model (that also is available as a separate Property Model Calculator model)

References

- Morral, J. E. & Purdy, G. R. “Particle coarsening in binary and multicomponent alloys,” *Scr. Metall. Mater.* 30, 905–908 (1994).

- Andersson, J. & Ågren, J. Models for numerical treatment of multicomponent diffusion in simple phases. *J. Appl. Phys.* 72, 1350–1355 (1992).

Equilibrium Model

The Equilibrium model calculates the equilibrium for the given conditions. Optionally define additional **Function Definitions**. All quantities that normally can be obtained from an equilibrium calculation can also be obtained when plotting the results, as well as the defined functions.

Equilibrium Calculator

An Equilibrium Calculator allows you to set the conditions for, and perform, a calculation. The Configuration window for an Equilibrium Calculator has these tabs:

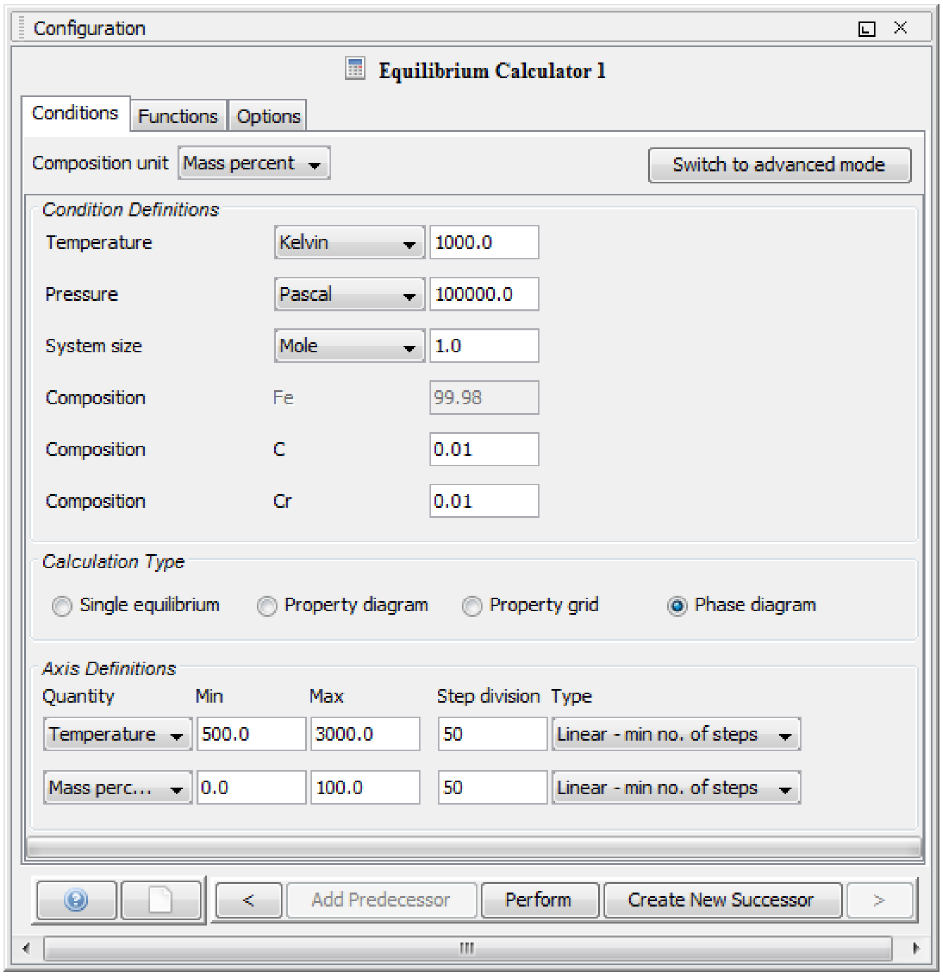
- **Conditions**: Set the conditions for your calculation that define the stepping or mapping axis variables. This tab can be viewed in a simplified mode and in an advanced mode. See *Setting Equilibrium Calculator Conditions* on the next page.
- **Functions**: Define your own quantities and functions, which you then can calculate and plot. See *Calculating and Plotting Functions* on page 77.
- **Options**: Modify numerical settings that determine how equilibria are calculated, as well as how stepping and mapping calculations are performed.

The **Options** tab is where you can locally define specific Equilibrium Calculator settings. These are the same settings described in *Global Settings: Calculation (Equilibrium Calculator)* on page 196.

See *Creating Activities and Successors* on page 30 for a list of possible successors and predecessors for this activity. An Equilibrium Calculator that is the successor of another Equilibrium Calculator inherits all the Configuration window settings of the predecessor.

For an example of how serially coupled Equilibrium Calculators can be used, see example 6 in *Graphical Mode Example Collection* on page 9.

Configuration Window



Equilibrium Calculator 1

Composition unit: Mass percent

Condition Definitions

Temperature	Kelvin	1000.0
Pressure	Pascal	100000.0
System size	Mole	1.0
Composition	Fe	99.98
Composition	C	0.01
Composition	Cr	0.01

Calculation Type

○ Single equilibrium ○ Property diagram ○ Property grid ● Phase diagram

Axis Definitions

Quantity	Min	Max	Step division	Type
Temperature	500.0	3000.0	50	Linear - min no. of steps
Mass perc...	0.0	100.0	50	Linear - min no. of steps

Setting Equilibrium Calculator Conditions

Conditions and axis variables for the Equilibrium Calculator are set in the Conditions tab of the Configuration window. The tab can be viewed in two modes: simplified (the default) or advanced.

The conditions to set depend on the type of calculation.

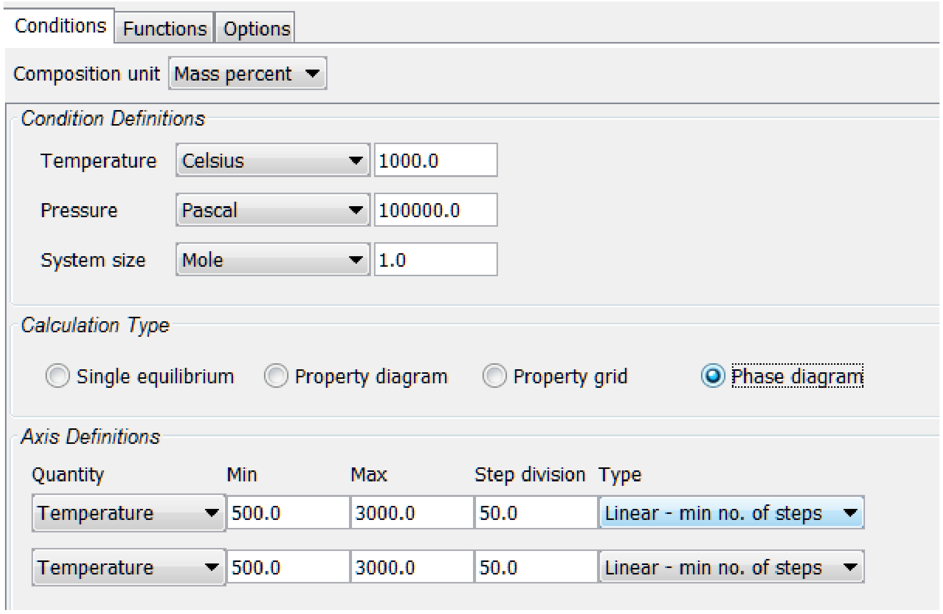
See *Graphical Mode Example Collection* on page 9: Example 1 is a single-point equilibrium calculation; Example 2 is a stepping calculation; Example 5 is a mapping calculation.

In advanced mode, you can add and remove conditions as well as set additional axis definitions. However, the number and types of conditions set must still conform to the Gibbs' phase rule. The **Number of missing conditions is** field, at the top of the tab shows how many conditions that you have left to set. If the number is negative, then that number of conditions need to be removed.

Setting Conditions for Simplified Mode

The following table briefly describes what you can set on the **Conditions** tab in simplified mode. Click **Switch to advanced mode** for more options.

The Conditions Tab



Composition unit: Mass percent

Condition Definitions

Temperature	Celsius	1000.0
Pressure	Pascal	100000.0
System size	Mole	1.0

Calculation Type

○ Single equilibrium ○ Property diagram ○ Property grid ● Phase diagram

Axis Definitions

Quantity	Min	Max	Step division	Type
Temperature	500.0	3000.0	50.0	Linear - min no. of steps
Temperature	500.0	3000.0	50.0	Linear - min no. of steps

Conditions Tab, Simplified Mode Settings

These are the settings on the Equilibrium Calculator Conditions tab in Simplified Mode.

Setting or Condition	Options
Composition unit	Choose from **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.
Condition Definitions	Specify the values (and units) of the state variables: **Temperature**, **Pressure**, and **System size**.
Calculation Type	**Single equilibrium** (no axes), **Property diagram**, **Property grid** or **Phase diagram**. For the **Single** calculation type no further settings are required. The results from this calculation are displayed in the **Event Log** .
Axis Definitions	**Property diagram**: Define the axis variable using these fields and menus: **Quantity**, **Min**, **Max**, **Step division** and **Type**. **Property grid**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max** and **Number of steps**. **Phase diagram**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max**, **Step division** and **Type**.

Setting or Condition	**Options**
	If the Equilibrium Calculator already has a Plot Renderer as a successor and you change the stepping/mapping quantities, then the quantities represented on the X- and Y-axis are automatically updated in the Plot Renderer.
Number of steps (Property grid)	Set a fixed **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point an equilibrium is calculated.
Type and Step division (Property diagram and Phase diagram)	**Type** options: Linear - min no. of steps, Linear - max step size and Logarithmic - scale factor. For Linear - min no. of steps, the **Step division** value specifies a minimum number of steps that is calculated between the minimum and maximum value during the stepping/mapping operation. For Linear - max step size, the **Step division** sets the maximum size of each step.For Logarithmic - scale factor, **Step division** specifies the scale factor of a logarithmic function that distributes the steps from the initial equilibrium to the minimum and maximum values defined.

Calculating with a Fixed Phase (Advanced Mode)

This describes how to use the advanced mode to set a phase to be fixed at a certain amount. This allows you to, for example, find out at what temperature a material starts to melt. If you set the phase to be fixed to liquid phase at zero amount, and do not define the temperature state variable, then you can calculate at what temperature the material enters a state where the liquid phase is no longer zero (that is, when it starts to melt).

How to Calculate with a Fixed Phase

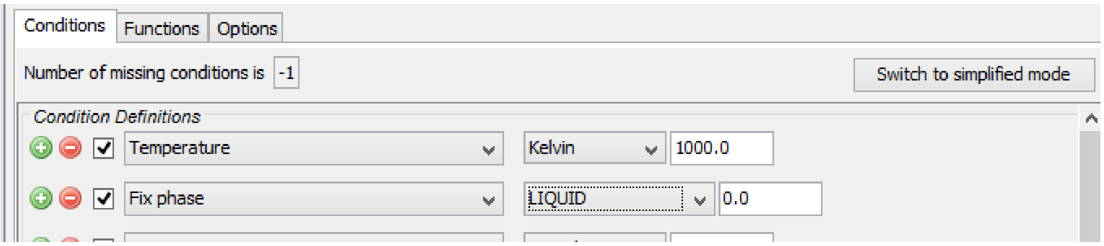
> For a fixed phase equilibrium calculation, it is recommended to serially couple the Equilibrium Calculators. This is where one Equilibrium Calculator activity is the successor to another Equilibrium Calculator activity that performs an ordinary equilibrium calculation, and then, for the condition you are interested in, you make a rough estimate of the value. This gives the fixed phase calculation better starting values.

1. Right-click a node that can add an Equilibrium Calculator to your project. See *Creating Activities and Successors* on page 30 for a list.
2. In the **Project** window, click the **Equilibrium Calculator** activity node.

3. In the **Configuration** window, click **Switch to advanced mode**.

If the **Default calculation mode** is globally set to **Advanced** then by default the Configuration window is already in advanced mode. See *Changing Global Settings* on page 189.

4. Under **Condition Definitions**, click the **Add quantity** button.
5. Select **Fix phase** from the first menu.
6. Select the phase that you want to fix in the second menu, and set the amount of that phase you want to fix the phase to. For example, if you want to know when your material starts to melt, set the phase to **LIQUID** and the value to **0.0**:



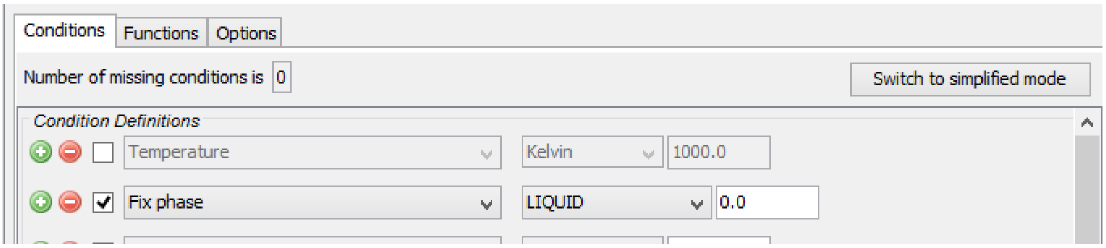
Number of missing conditions is -1

☑ Temperature Kelvin 1000.0

☑ Fix phase LIQUID 0.0

Above the condition definitions, the **Number of missing conditions is** field is probably **-1**. This means that you must remove one condition.

7. To remove a condition, either click the remove button, or click to clear the check-box. For example, if you want to know at what temperature your material starts to melt, then you cannot have a fixed temperature, in which case the temperature condition is not selected:



Number of missing conditions is 0

☐ Temperature Kelvin 1000.0

☑ Fix phase LIQUID 0.0

The **Number of missing conditions is** field displays **0**. When you have set all your conditions, you can perform the Equilibrium Calculator (now or later).

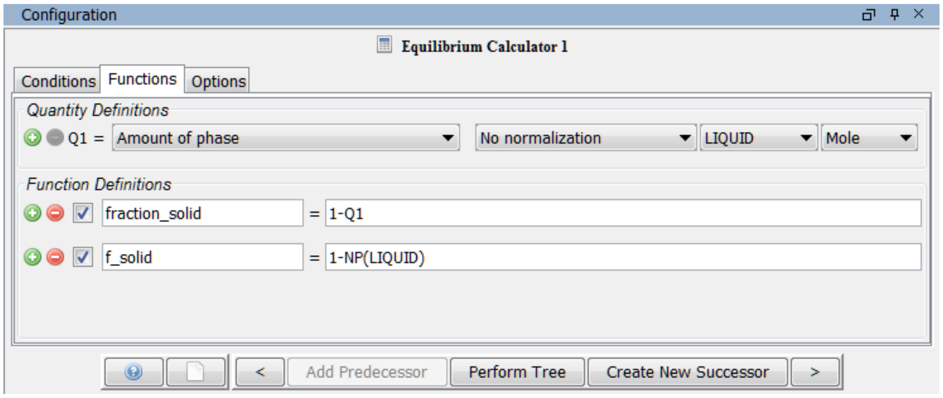
Calculating and Plotting Functions

The **Functions** tab allows you to define your own functions that can be plotted in a Plot Renderer.

For an example of how you can use functions that you yourself define, see example 7 in *Graphical Mode Example Collection* on page 9.

How to Calculate and Plot Functions

1. Create an **Equilibrium Calculator** node and click it in the **Project** window.
2. In the **Configuration** window click the **Functions** tab.
3. Under **Quantity Definitions**, define **Q1**. Click the add ⊕ button to **Add a new quantity**. Then from the lists, choose the variable for each quantity to define. The quantities are called **Q1**, **Q2**, **Q3** and so on. In this example, the quantity **Q1** is defined as the **Amount of phase**, with **No normalization**, **LIQUID** in **Mole** units.



Quantity Definitions

Q1 = Amount of phase | No normalization | LIQUID | Mole

Function Definitions

☑ fraction_solid = 1-Q1

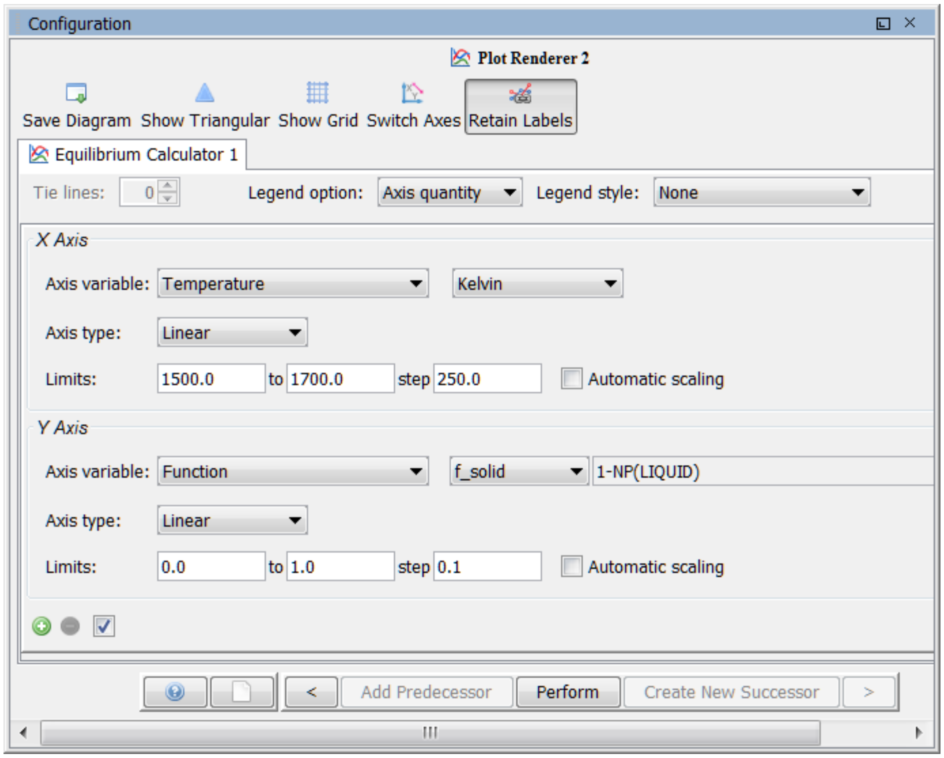
☑ f_solid = 1-NP(LIQUID)

4. Under **Function Definitions**, click the add ⊕ button to add a new function. In the left field edit the default name of each function and enter the function itself in the right field after the equal sign. In this example, the quantity defined as Q1 is renamed to **fraction_solid**, which gives as its output the fraction of solid phase (**1-Q1**).

You can also use Console Mode syntax when entering the function. For example, the function above can be entered as `1-NP(LIQUID)`.

5. To plot the defined function, right-click **Equilibrium Calculator** and choose **Create new successor→Plot Renderer**.
6. Click the **Plot Renderer** node. In the tab for the Equilibrium Calculator that contains the function, set an **Axis variable** to **Function**, then from the menu select the defined function. In this example the Y-axis is set to plot the value of the function **fraction_solid**.

   When run, the Plot Renderer plots the value of the function.



Tie lines: 0

Legend option: Axis quantity

Legend style: None

X Axis

Axis variable: Temperature, Kelvin

Axis type: Linear

Limits: 1500.0 to 1700.0 step 250.0 ☐ Automatic scaling

Y Axis

Axis variable: Function, f_solid, 1-NP(LIQUID)

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☐ Automatic scaling

☑

Precipitation Calculator

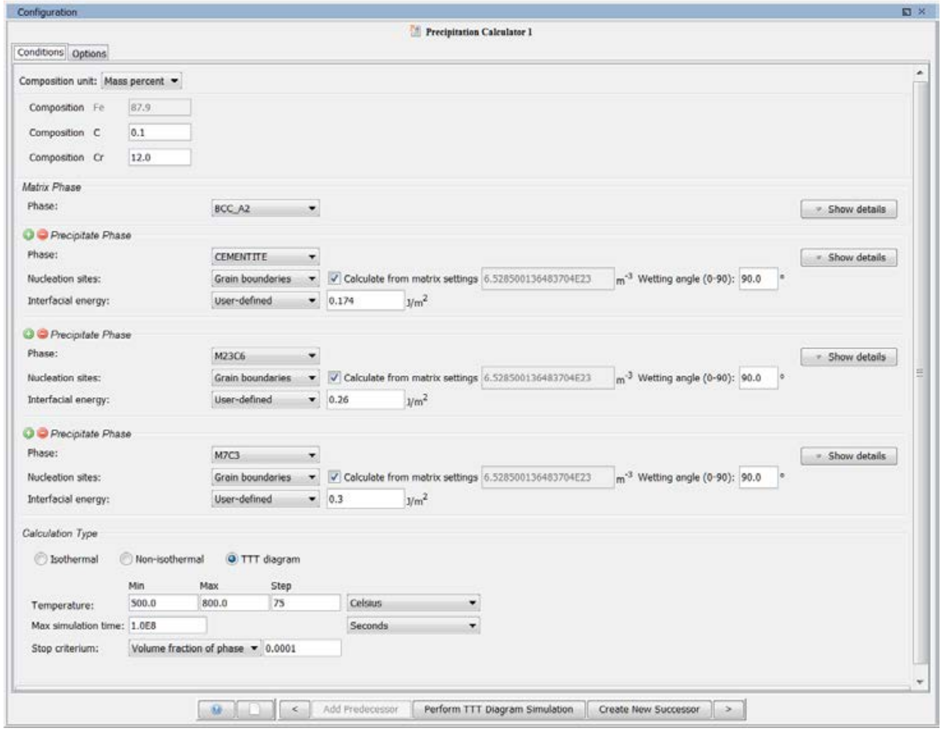
The Precipitation Calculator is available with two components if you do not have the additional Precipitation Module (TC-PRISMA) license. With the add-on module you can use all available components.

A Precipitation Calculator allows you to set the conditions for, and perform, a precipitation calculation. The Configuration window for a Precipitation Calculator has these tabs:

- **Conditions**: Set the conditions for your calculation that define the Matrix and Precipitate phases. Choose the Calculation Type.
- **Options**: Modify Numerical Parameters that determine how the conditions are calculated. The Growth rate model can be viewed in Simplified or Advanced mode.

Configuration Window

Example



Composition unit: Mass percent
Composition Fe 87.9
Composition C 0.1
Composition Cr 12.0

Matrix Phase
Phase: BCC_A2

Precipitate Phase
Phase: CEMENTITE
Nucleation sites: Grain boundaries ☑ Calculate from matrix settings 6.528500136483704E23 m^{-3} Wetting angle (0-90): 90.0 °
Interfacial energy: User-defined 0.174 J/m^2

Precipitate Phase
Phase: M23C6
Nucleation sites: Grain boundaries ☑ Calculate from matrix settings 6.528500136483704E23 m^{-3} Wetting angle (0-90): 90.0 °
Interfacial energy: User-defined 0.26 J/m^2

Precipitate Phase
Phase: M7C3
Nucleation sites: Grain boundaries ☑ Calculate from matrix settings 6.528500136483704E23 m^{-3} Wetting angle (0-90): 90.0 °
Interfacial energy: User-defined 0.3 J/m^2

Calculation Type
○ Isothermal ○ Non-isothermal ● TTT diagram

	Min	Max	Step	
Temperature:	500.0	800.0	75	Celsius
Max simulation time:	1.0E8			Seconds
Stop criterium:	Volume fraction of phase	0.0001		

Conditions Tab Settings

These are the settings on the Precipitation Calculator Conditions tab.

Setting or Condition	Options
Composition unit	Choose from **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.
Matrix Phase	Specify the **Phase**. Click **Show Details** for more settings.
Precipitate Phase	Specify the **Phase**, **Nucleation Sites**, and **Interfacial energy**. Click **Show Details** for more settings.
Calculation Type	Choose **Isothermal**, **Non-isothermal** or **TTT diagram**.

Matrix Phase

Phase: Choose a phase from the list. The list is based on the settings for the System Definer. When setting up your system, choose a matrix phase with kinetic data available in the database.

Only phases with kinetic data can be selected as the matrix phase. If the list is empty, go to the System Definer to make sure that both types of databases are selected and defined. See "System Definer" in the *Thermo-Calc User Guide* or search the Online Help.

Click **Show details** to view these additional settings:

- **Molar volume**: Choose the default to take the value from the **Database** or **User-defined** to enter another value. **Database** is available in the list when the molar volume for the phase is defined in the thermodynamic database.
- **Grain radius**: Enter a numerical value and choose a unit from the list.
- **Grain aspect ratio**: Enter a numerical value.
- **Dislocation density**: Enter a numerical value.
- **Mobility enhancement prefactor**: Enter a numerical value.
- **Mobility enhancement activation energy**: Enter a numerical value.

Precipitate Phase

Phase: Choose a phase from the list. The list is based on the settings for the System Definer.

The phases available to choose have both thermodynamic and kinetic data. If the list is empty, go to the System Definer to make sure that both types of databases are selected and defined. See "System Definer" in the *Thermo-Calc User Guide* or search the Online Help.

Nucleation sites: Choose one of the following from the list.

- **Bulk**, **Grain boundaries**, **Grain edges**, **Grain corners**, or **Dislocations**. Click to select the **Calculate from matrix settings** check box if you want to calculate the number density of sites.
- For Grain boundaries, Grain edges and Grain corners, enter the **Wetting angle** in addition to the matrix settings.
- To enter a specific value for the number of nucleation sites, deselect the check box.

Interfacial energy: Choose **Calculated** to use the estimated value and then enter a different **prefactor** value if you want to adjust the estimated value. You can also choose **User defined** to enter a value in J/m^2.

Click **Show details** to view these additional settings:

- **Molar volume**: Choose the default to take the value from the **Database** or **User-defined** to enter another value. **Database** is available in the list when the molar volume for the phase is defined in the thermodynamic database.
- **Phase boundary mobility**: Enter a numerical value.
- **Phase energy addition**: Enter a numerical value.

- **Approximate driving force**: Select the check box to include this if simulations with several compositions sets of the same phase create problems.

Calculation Type

Isothermal

Use an **Isothermal** calculation type to do a precipitation simulation at constant temperature.

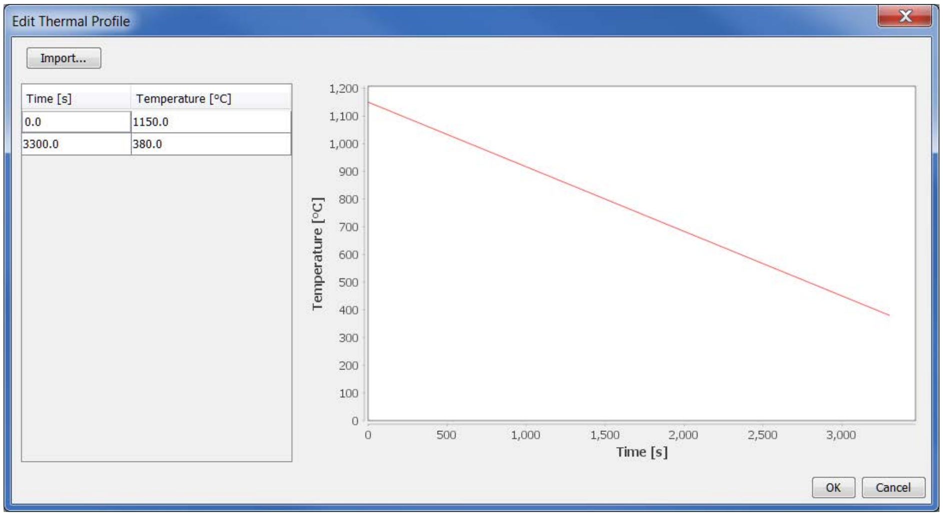
For the **Isothermal** calculation type, enter a **Temperature** and **Simulation time**.

Non-Isothermal

For the **Non-isothermal** calculation type, select a **Temperature unit** and **Time unit** from the lists. Enter a value for the **Simulation time**.

Click **Thermal Profile** to define the heat treatment schedule. Here the **Temperature** and **Time** coordinates of thermal profile points are entered. A minimum of two points is required. You can also click **Import** to add your own thermal profile from an Excel spreadsheet.

Edit Thermal Profile Window



Time [s]	Temperature [°C]
0.0	1150.0
3300.0	380.0

TTT-Diagram

Use a **TTT-diagram** calculation type to do a a precipitation simulation of the time-temperature-transformation (TTT).

For the **TTT diagram** calculation type , enter **Min**, **Max**, and **Step** values for the **Temperature** and choose a **Unit** from the list.

Max simulation time: Enter a numerical value and choose a **Unit** from the list.

Stop criterium: Choose **Volume fraction of phase** or **% of equilibrium fraction** and then enter a numerical value in the field. For each temperature, the simulation stops when the stop criterium is fulfilled or if the maximum simulation time is reached, whichever happens first.

Options Tab Settings

These are the settings on the Precipitation Calculator Options tab.

Settings

Growth Rate Model

Choose from **Simplified** (the default) or **Advanced**.

Numerical Parameters

Enter numerical values for the following as required.

- **Max time step fraction**: The maximum time step allowed for time integration as fraction of the simulation time.
- **No. of grid points over one order of magnitude in radius**: Default number of grid points for every order of magnitude in size space.
- **Max no. of grid points over one order of magnitude in radius**: The maximum allowed number of grid points in size space.
- **Min no. of grid points over one order of magnitude in radius**: The minimum allowed number of grid points in size space.
- **Max relative volume fraction of subcritical particles allowed to dissolve in one time step**: The portion of the volume fraction that can be ignored when determining the time step.
- **Max relative radius change**: The maximum value allowed for relative radius change in one time step.
- **Relative radius change for avoiding class collision**: Set a limit on the time step.
- **Max overall volume change**: This defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step.
- **Max relative change of nucleation rate in logarithmic scale**: This parameter ensures accuracy for the evolution of effective nucleation rate.
- **Max relative change of critical radius**: Used to place a constraint on how fast the critical radium can vary, and thus put a limit on time step
- **Min radius for a nucleus to be considered as a particle**: The cut-off lower limit of precipitate radius.
- **Max time step during heating stages**: The upper limit of the time step that has been enforced in the heating stages.

Plot Renderer

The Plot Renderer displays results from the various calculator activities .

The available Plot Renderer functionality varies by calculation type. For example:

- If you choose a *Property grid* (Equilibrium Calculator) or *Grid* (Property Model Calculator) calculation type, select a **Plot type** and whether to **Interpolate** the data or not.
- For a Property Model Calculator *Uncertainty* calculation type, you choose an **Axis type**: **Frequency**, **Histogram** or **Normal probability**. For other calculators (e.g. Equilibrium, Binary, and Scheil) there are different axis types available such as **Linear**, **Logarithmic**, **Logarithmic 10**, and **Inverse**.

The Plot Renderer is used to set the plotting axis variables for a property diagram and phase diagram.

If you are plotting a Property grid (Equilibrium Calculator) or Grid (Property Model Calculator) then the X- and Y-axes always represent the quantities that define the stepping axes, but you need to set a variable for the Z-axis (the axis perpendicular to the plane defined by the X- and Y-axes).

Also see *Creating Activities and Successors* on page 30 for a list of possible successors and predecessors for this activity.

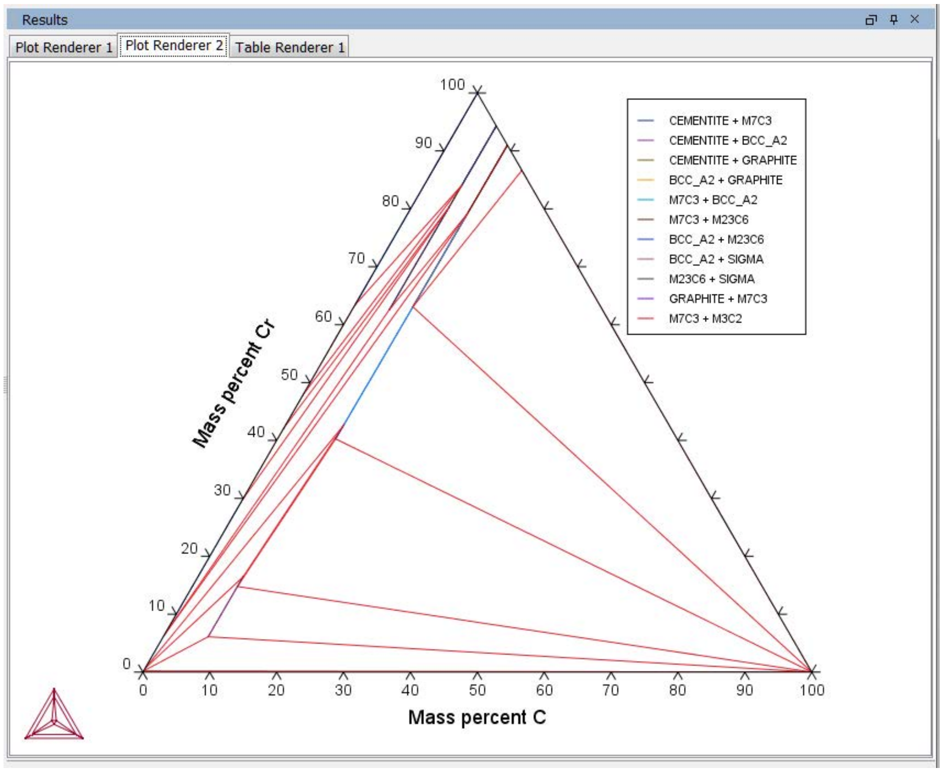
The configurations that can be set in the Configuration window for a Plot Renderer vary depending on the kind of predecessor it is created from.

Plot Several Calculations in One Diagram

A Plot Renderer can have several predecessors (if you want to plot several calculations in the same diagram), in which case there are several tabs in the Configuration window, one for each predecessor.

Several Plot Renderer activities (as well as Table Renderer activities) can be shown in the Results window as different tabs. The figure is from Graphical Mode example 4 .

Also see *Plotting Several Calculations in One Diagram* on page 97 for details.

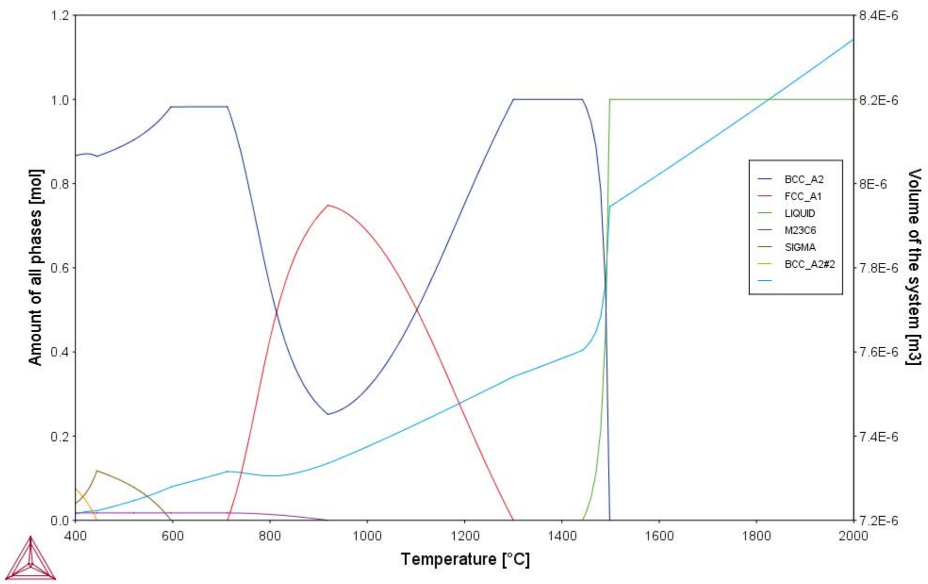


Add Axes to Diagrams

You can add additional X- and/or Y-axes to a plot to compare two or more variables at the same time as in the figure.

Also see *Adding Axes to a Diagram* on page 98 for details.

Two variables plotted on the Y-axis.



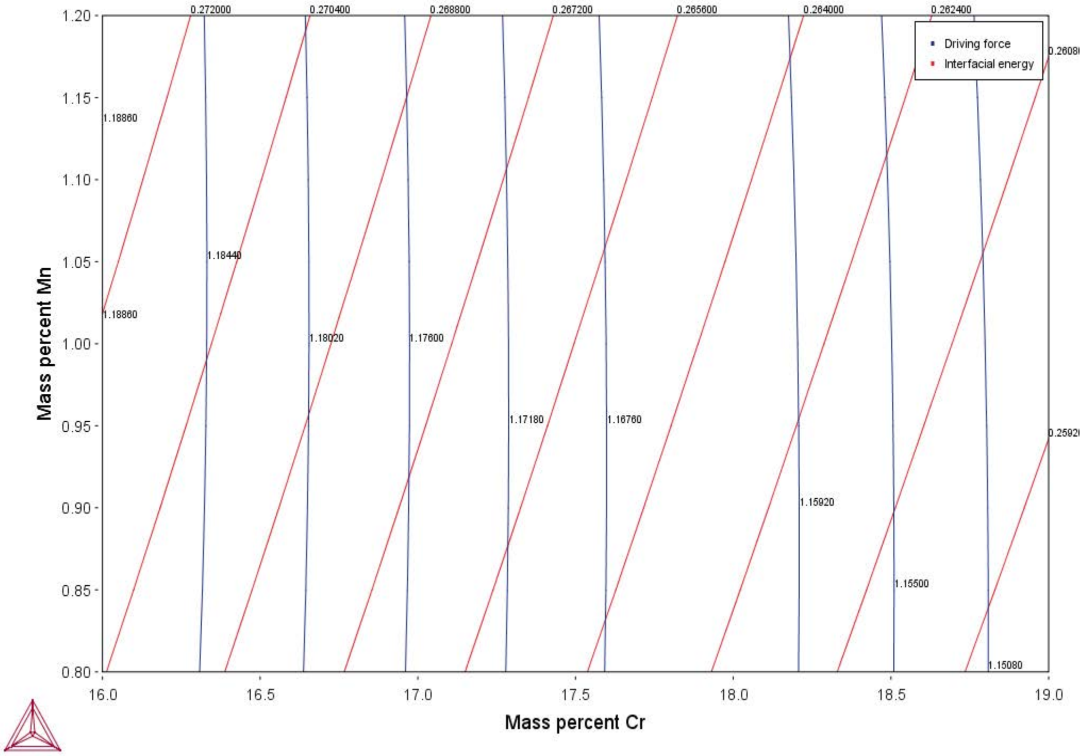
Merge Results in One Diagram

You can merge (or overlay) calculated results for several variables into one diagram. This is similar to adding an axis, but instead of displaying different variables along the X- and/or Y-axes, the same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).

As in the figure (from example 12 in Graphical Mode Examples), the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).

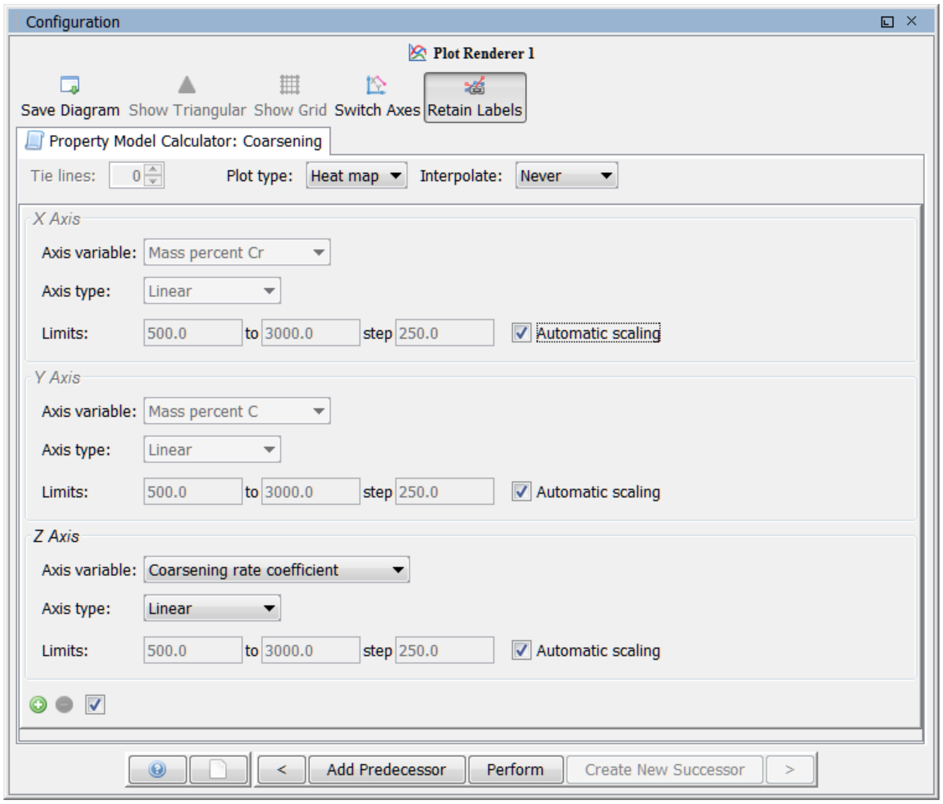
Also see *Merging Plots into One Diagram* on page 100 for details of how to combine diagrams.

A contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.



Configuration Window

The Configuration window has different options available based on its predecessor. The following is an example of the Configuration window for a Plot Renderer that is the successor to an Equilibrium Calculator. The options along the top are available for most of the calculation types (e.g. phase diagrams, property diagrams, min/max, uncertainty and so forth). For an Equilibrium Property Grid calculation type and a Property Model Calculator Grid calculation you can choose a **Plot type**.



Tie lines: 0 Plot type: Heat map Interpolate: Never

X Axis

Axis variable: Mass percent Cr

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

Y Axis

Axis variable: Mass percent C

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

Z Axis

Axis variable: Coarsening rate coefficient

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

Configuration Settings

Setting/Button	Description
Save Diagram	Save the plot diagram.
Show Triangular	Display the diagram in triangular form, with the X-axis along the base and the Y-axis along the left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
Show Grid	Overlay a grid on the diagram.
Switch Axes	Show the plotting X axis variable on the diagram's Y-axis, and the Y axis variable on the diagram's X-axis.
Retain Labels	Toggle the default to keep labels displaying on the plot. By default labels are retained.

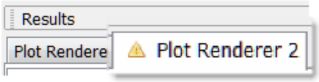
Setting/Button	Description
Tie lines	Select how many tie lines to be plotted in the diagram. Every nth number of tie line is plotted, where n is the number set here. Consequently, the higher the number, the fewer the number of plotted tie lines in the diagram. This setting is not available if the Plot Renderer is a successor to a Precipitation Calculator, Scheil Calculator or to an Equilibrium Calculator where only one axis is defined and varied (that is, an Equilibrium Calculator that has performed a stepping calculation).
Legend option	Select whether the diagram's legend displays the Stable phases, the Axis quantity, or choose Off for no legend.
Legend style	You can select a Legend style for the **Stable phases** or **Axis quantity** selected for **Legend option**. Choose **None**, **All**, **Constitution description**, or **Ordering description**. Also see *About Legend Styles* on page 92.
Plot type (property grid or grid)	This menu is available if the Plot Renderer is a successor to either an Equilibrium Calculator that is set up to calculate a *Property grid* or a Property Model Calculator that is calculating a *Grid*. On a **Heat map** diagram, each equilibrium calculation in the grid is represented by a colour-coded pixel, where dark red represents the highest Z-axis variable value and dark blue represents the lowest Z-axis variable value. On a **Contour** diagram, Z-axis variable values are traced with curves in different colours (in the same way that height values are traced with curves on a topographical map). From the **Interpolate** list, choose to interpolate data **Never** (the default), **Once**, **Twice** or **3 times**. This means points are put in between calculated points in the grid and interpolated instead of calculated in the calculation engine.
Interpolate (property grid or grid)	Choose how many points of data to interpolate on a grid or property grid to improve curve smoothness – **Never**, **20x20**, **50x50**, or **100x100**. Try different settings for your own set of data.

Setting/Button	Description
Axis variable	Set the state variable you want plotted along the X-axis and the Y-axis. If the stepping/mapping variables are changed in the Equilibrium Calculator that precedes the Plot Renderer, then the variables to be plotted along the diagram’s X- and Y-axis are automatically updated to the appropriate quantities. For a Precipitation Calculator: • Select the **Separate multimodal PSD** check box to enter settings for **Points**, **Excess kurtosis**, **Valley depth ratio** and **Minimum peak**.
Axis type	Select what type of scale to use on the axis. Choose between **Linear**, **Logarithmic**, **Logarithmic 10** or **Inverse**.
Limits	Specify the range along the axis that is shown in the plot by setting the minimum and maximum values of the axis variable. You can also determine the step size between the tick marks along each axis. Alternatively, select Automatic scaling.
Contour values and Use custom contour values (Z-axis, contour plots).	The **Use custom contour values** check box is available when **Contour** is selected as the **Plot type**. Select this check box to enter one or a series of numbers in the **Contour values** field. Numbers can be separated by a space, colon (:), semicolon (;) or comma (,).
Unit (*Time X Axis*)	For a Precipitation Calculator choose a **Unit** - **Seconds**, **Hours**, or **Days**.
Add an axis ⊕ and Remove this axis ⊖ buttons.	Use these buttons to add additional X- and/or Y-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the Z-axis. See Adding Axes to a Diagram and Merging Plots into One Diagram for details.

Plot Status Marker

If you have plotted a diagram and then modify something in the tree that the Plot Renderer is associated with, then a notification sign—an exclamation mark enclosed in a yellow triangle—is shown in the Plot Renderer’s tab.

Also see *Node Status Markers* on page 41.



About Legend Styles

There are a variety of legend styles you can use to display detail about the phases.

The same legend styles are available for both Graphical Mode and Console Mode plots. For Console Mode, use the command CHANGE_LEGEND in the *Thermo-Calc Console Mode Command Reference Guide*.

In Graphical Mode the label styles are defined when using the *Plot Renderer* on page 84. You can select a **Legend style** for the **Stable phases** or **Axis quantity** selected for **Legend option**.

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

If constituent description is included in the legend, then for each equilibria along a line in the diagram, the largest constituent fractions are summed until they are equal or greater than 0.6. This is done separately for each sublattice. If the equilibria along the line gets different sets of constituents these are all appended to the list for that sublattice.

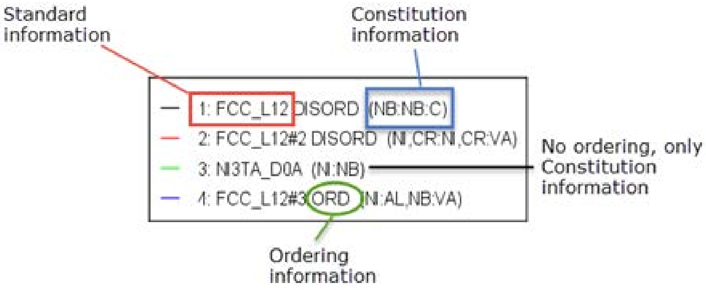
The ordering description is only printed for partitioned phases (phases that have a disordered contribution) that begins with at least two identical sublattices (sublattices where the set of constituents are identical). `DISORD` (disordered) is shown if site fractions are identical between identical constituents on all identical sub lattices (with an error margin) otherwise `ORD` (ordered) is shown in the legend.

If ordering between equilibria in a line are different, then `ORD + DISORD` is shown in the legend.

Legend Examples

To show the differences between labels, the following uses the same example file that creates Figure 6 in TCNi8 database extended information document (found on the Thermo-Calc website).

When **All** is selected for this specific example the label includes the following:



Specifically:

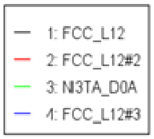
- There are two disordered FCC phases (matrix and carbide), one ordered FCC (gamma prime), plus a phase NI3TA_D0A (called Delta in Ni-alloys).
- ORDERING shows the different FCC phases.
- CONSTITUTION shows that FCC_L12#1 is NbC, FCC_L12#2 is matrix with Ni and Cr as major constituent, FCC_L12#3 is Ni3Al with Nb addition and NI3TA_D0A is Nb-rich (eg. Ni3Nb).

Label Style Choice Examples

These examples are for each label style choice - None, All, Constitution or Ordering

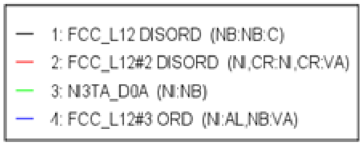
The instructions are for when you are setting the options using the Plot Renderer. In Console Mode, you choose the options (`ALL`, `NONE`, `CONSTITUTION`, or `ORDERING`) after the command CHANGE_LEGEND.

When **None** is selected the legend includes the standard information about the phases.



— 1: FCC_L12
— 2: FCC_L12#2
— 3: NI3TA_D0A
— 4: FCC_L12#3

When you select **All** the **Constitution description** and the **Ordering description** (when there is ordering) are included.

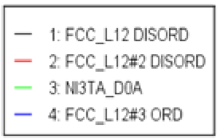


— 1: FCC_L12 DISORD (NB:NB:C)
— 2: FCC_L12#2 DISORD (NI,CR:NI,CR:VA)
— 3: NI3TA_D0A (NI:NB)
— 4: FCC_L12#3 ORD (NI:AL,NB:VA)

When you select **Constitution description**, this is added to the standard description.

— 1: FCC_L12(NB:NB:C)
— 2: FCC_L12#2(NI,CR:NI,CR:VA)
— 3: NI3TA_D0A(NI:NB)
— 4: FCC_L12#3(NI:AL,NB:VA)

When you select **Ordering description** and when there is ordering, this is added to the standard description.

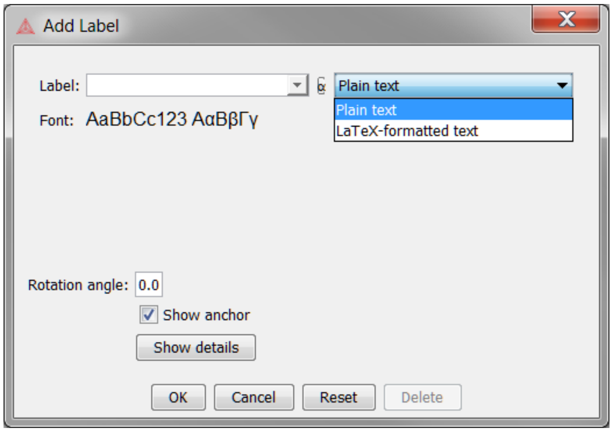


— 1: FCC_L12 DISORD
— 2: FCC_L12#2 DISORD
— 3: NI3TA_D0A
— 4: FCC_L12#3 ORD

Adding and Editing Plot Labels

To add a label text at a certain point in a plot, right click the point, and select **Add Label**. For phase diagrams, the program suggests a label that you can keep or edit. The suggested label specifies the names of the stable phases at the coordinate where you clicked. For all other plot types, you enter your own text, which can either be Plain text or LaTeX formatted text.

Add Label WIndow



Label Formatting

You can enter the label as **Plain text** or in **LaTeX-formatted text**. For **LaTeX-formatted text** enter or edit the text as required. For example, underscores (_) are added before the numbers to make subscripts in the label.

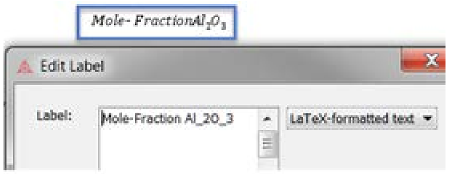
For a list of supported LaTeX commands, see: http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html.

By default when using LaTeX, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.

Entering a Mixture of Plain Text and Equations

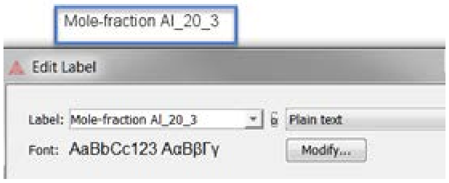
When you enter text using LaTaX formatted text it displays by default on the plot in italics and treats the text as an equation.

As in the following example, the top label does not display correctly because the label is a mixture of text (Mole-Fraction) and an equation (Al_2O_3). In the bottom image, when the same information is added as Plain text to the plot it now does not include the subscripts.



Label: Mole-Fraction Al_20_3

LaTeX-formatted text

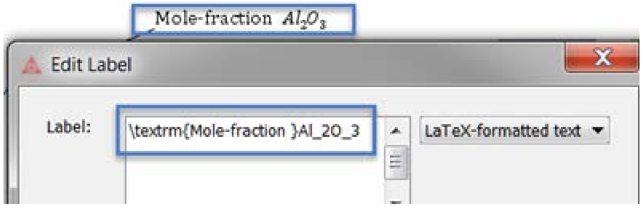


Label: Mole-fraction Al_20_3

Plain text

Font: AaBbCc123 AαBβΓγ

To add a mixture of plain text and equation text, you can exit math mode using the string `\textrm` followed by the text to display enclosed in curly brackets. For example `\textrm{Mole-fraction }Al_20_3` results in the label as shown:



Label: \textrm{Mole-fraction }Al_20_3

LaTeX-formatted text

In this example, you need to add a space at the end of fraction in order to separate the text from the equation part of the label.

When working in Console Mode, you can also use the above windows on the Console Results window to add and edit labels. In addition, you can use the ADD_LABEL_TEXT command described in the *Thermo-Calc Console Mode Command Reference*.

Rotation Angle and Show Anchor

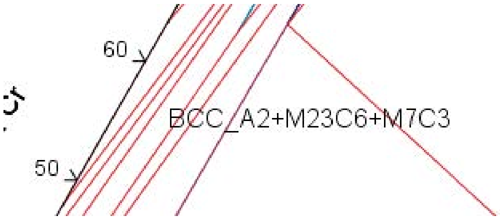
By default the **Show anchor** check box is selected, which includes an arrow from the label point to the coordinates.

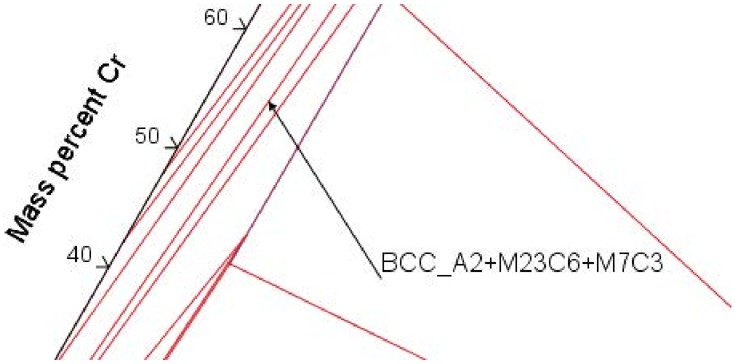
If you do not want the label oriented horizontally in the Plot Renderer tab, then specify the number of degrees of rotation in the **Rotation angle** field.

Click **OK** to add the label to the plot. You can also move a label by clicking and dragging it. The default anchor arrow is added to indicate the point that belongs to the label.

Moving Labels in a Plot

Drag and drop labels anywhere on the plot. The anchor arrow points to the point of origin.



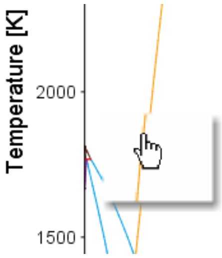


Changing the Plot Properties

For global changes to the default settings plots see *Global Settings: Graphical and Console Mode-Plotting* on page 202. The settings are the same but applied to all new plots.

To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included).

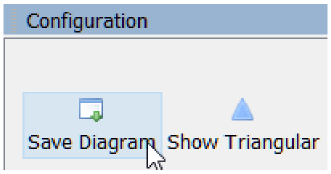
In the **Results** window, hover the mouse over a plot line. When it is over a line that can clicked the crosshair cursor turns into a pointing finger.



To prevent unintended edits, hold down <Ctrl> while moving the cursor around the plot to only display it as a crosshair.

Saving Plots

1. To save a diagram, at the top of the **Configuration** window click **Save Diagram**.



Or right-click the diagram in the **Results** window and select **Save As**.

2. In the **Save** window, navigate to where you want to save the plot, enter a **File name**, and choose the **File type** to save it in. Click **Save**.

Plotting Several Calculations in One Diagram

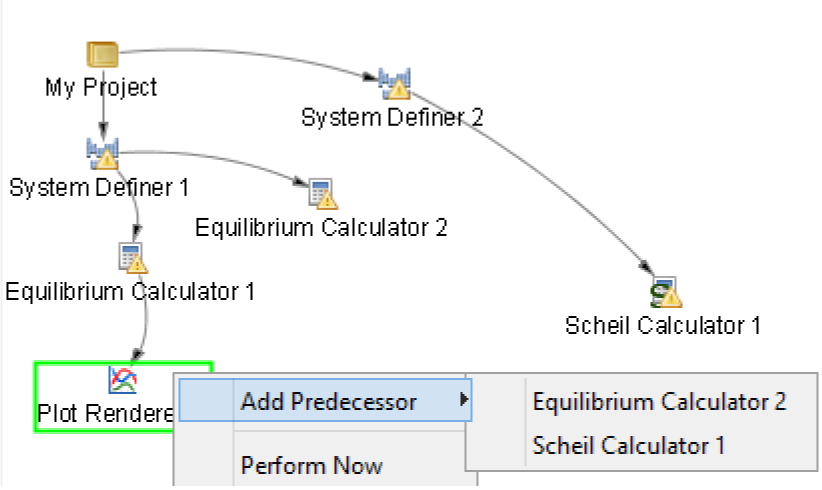
You can plot several calculations in the same diagram by adding extra predecessors to the Plot Renderer activity.

For an example of a project in which several calculations are plotted in one diagram, see example 5 in *Graphical Mode Example Collection* on page 9.

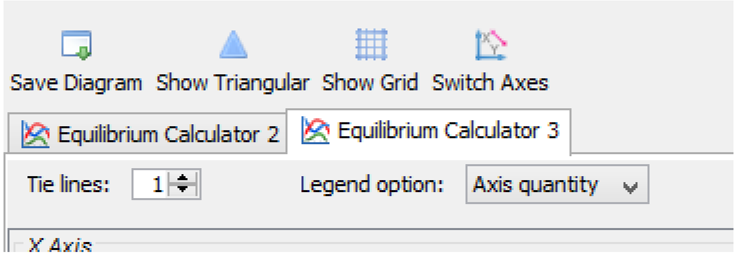
To plot several calculations in one diagram, you must have, in addition to the Plot Renderer's original predecessor, at least one available Plot Renderer predecessor in your project. The extra predecessor can be any of these: Equilibrium Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator or Experimental File Reader.

How to Plot Several Calculations in One Diagram

1. In the Project window click the **Plot Renderer** node.
2. In the **Configuration** window click **Add Predecessor**. Or right-click the **Plot Renderer** and choose **Add Predecessor**.



3. Select a predecessor. When added, the extra predecessor is linked to the Plot Renderer. On the Plot Renderer's Configuration window, the predecessors are shown as two tabs:

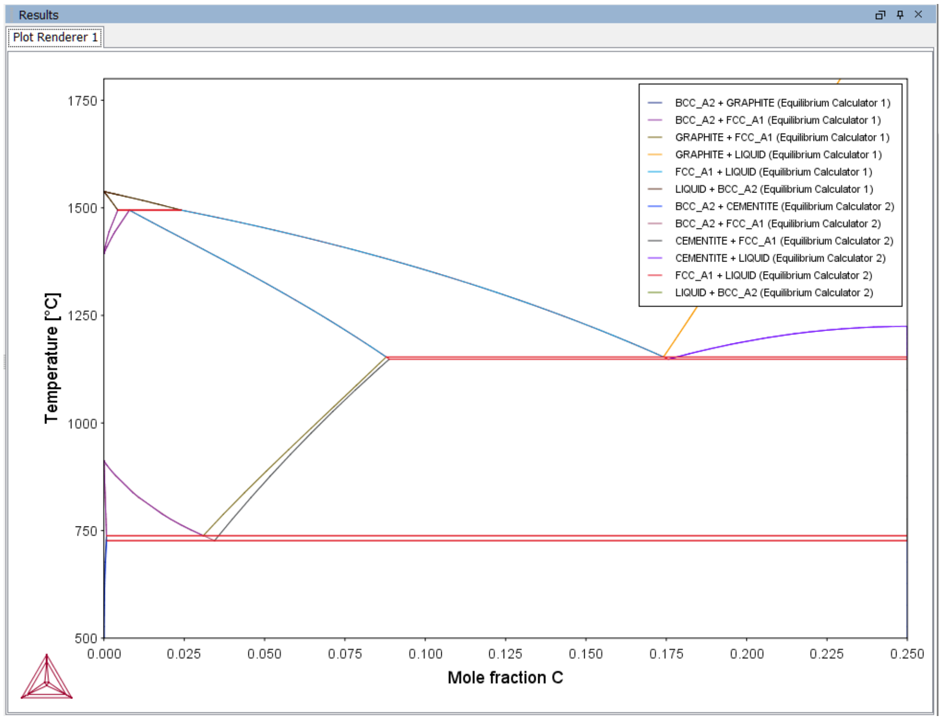


Tie lines: 1

Legend option: Axis quantity

4. Configure how you want each calculation plotted on the tabs in the **Configuration** window, then click to **Perform** the Plot Renderer activity.

The calculations are plotted in the same diagram in a tab in the **Results** window. If any of the axis variables of the plots differ, then the label and scale of all calculations are shown parallel to each other. The following screen shot shows a diagram in which two calculations with different plotting axes variables have been plotted.



Adding Axes to a Diagram

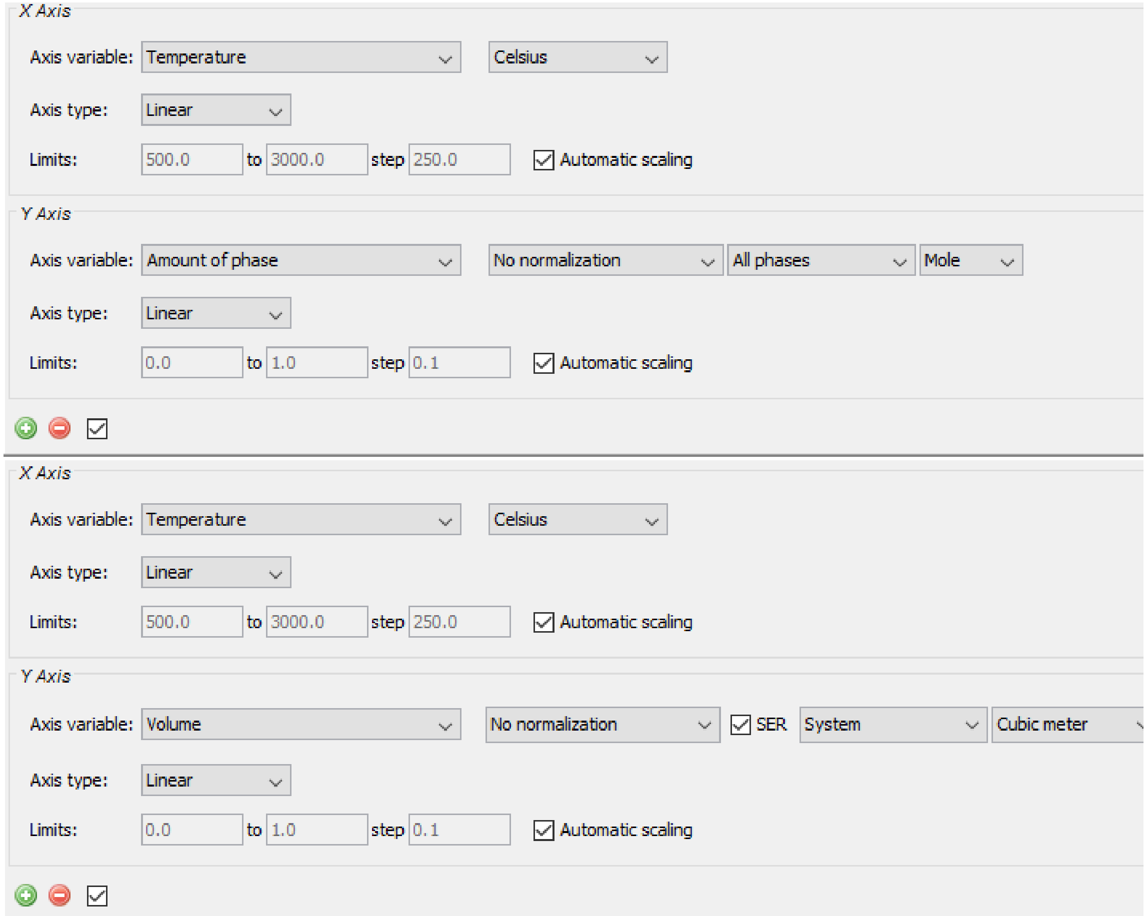
You can add additional *X*- and/or *Y*-axes to a plot to compare two or more variables at the same time.

1. In the **Project** window right-click the calculator node (e.g. an Equilibrium Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Available settings are based on the calculation type.
4. Click the **Add an axis** ⊕ button. A new settings section is added underneath.
5. From the *X Axis* and/or *Y Axis* sections define another **Axis variable** and choose an **Axis type**.

6. Click **Perform** to plot both variables on the selected axis, in this example, the Y-axis.

Axis Example

In this example **Amount of phase** and **Volume** are selected as the Y-axis variables and **Temperature** as the X-axis variable.



X Axis

Axis variable: Temperature | Celsius

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

Y Axis

Axis variable: Amount of phase | No normalization | All phases | Mole

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

⊕ ⊖ ☑

X Axis

Axis variable: Temperature | Celsius

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

Y Axis

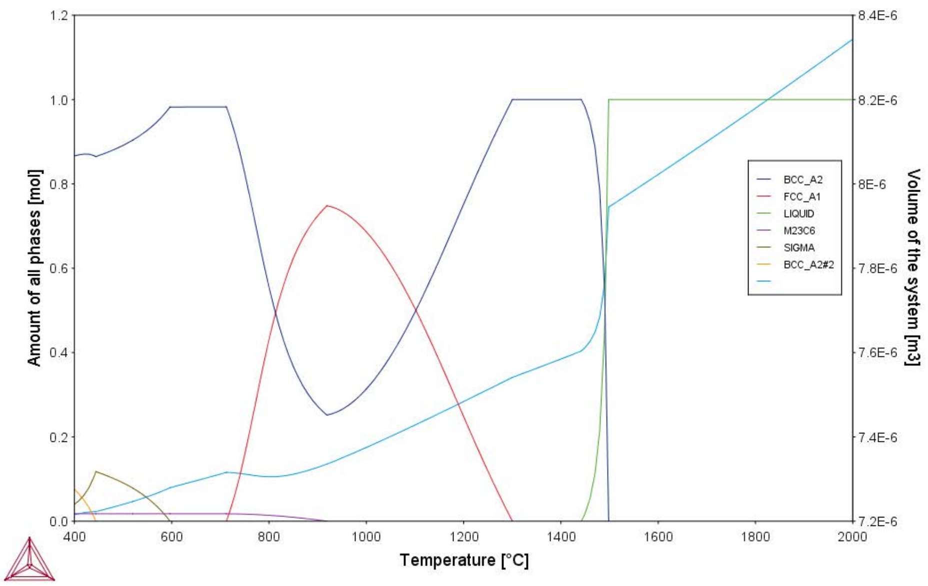
Axis variable: Volume | No normalization | ☑ SER | System | Cubic meter

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

⊕ ⊖ ☑

Plot Example



Merging Plots into One Diagram

You can merge (or overlay) calculated results for several variables into one diagram. The same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).

You cannot overlay heat map or frequency plots.

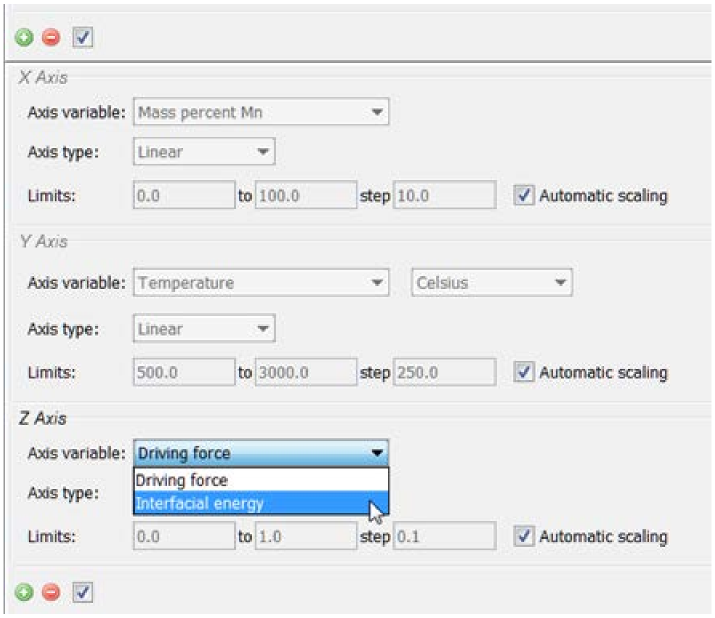
The following uses example 12 in Graphical Mode Examples to describe the steps to overlay two plots: the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).

1. In the **Project** window right-click the calculator node (e.g. Property Model Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Available settings are based on the calculation type.

   ### Example

   In this example the Property Model Calculator is set to a *Grid* calculation type.

   Choose **On** for the **Legend option** and **Contour** as the **Plot type**.



X Axis

Axis variable: Mass percent Mn

Axis type: Linear

Limits: 0.0 to 100.0 step 10.0 ☑ Automatic scaling

Y Axis

Axis variable: Temperature Celsius

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

Z Axis

Axis variable: Driving force

Driving force

Interfacial energy

Axis type:

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

4. Click the **Add an axis** ⊕button. A new axes settings section is added underneath.
5. From the *Z Axis* section choose the **Axis variable**. In this example, **Interfacial energy**.

6. Click **Perform** to plot both on the same diagram.

Plot Example

In this case, a contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.

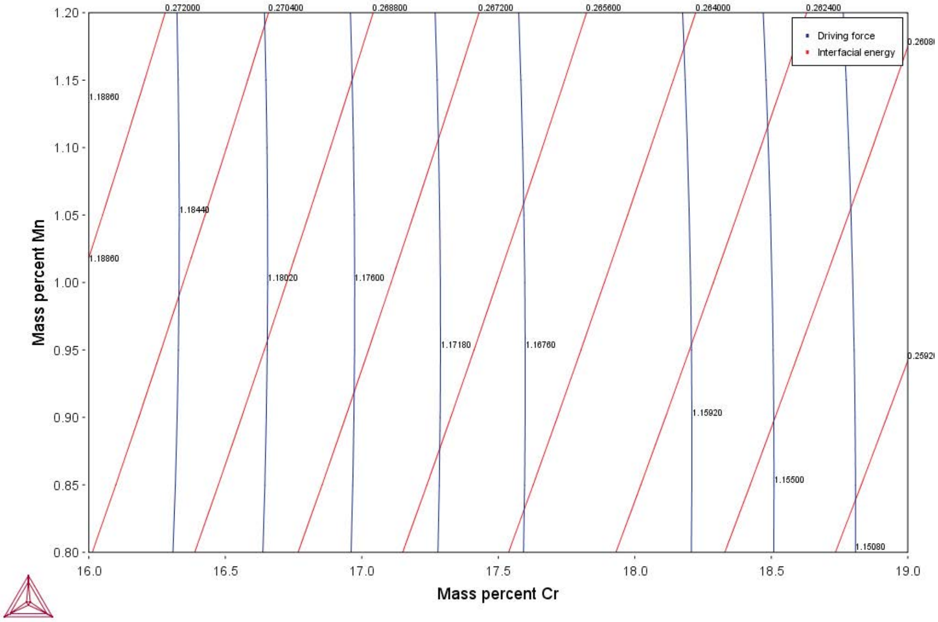


Table Renderer

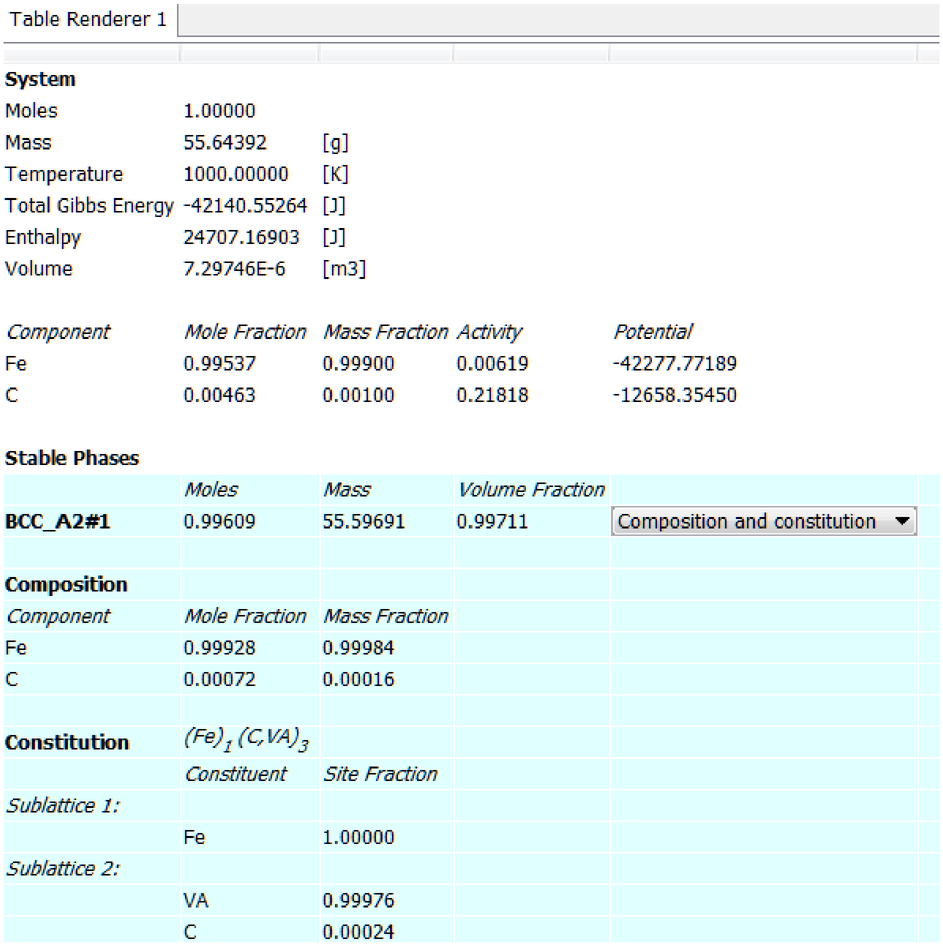
A Table Renderer visualizes calculation results in a table. Several Table Renderer activities (as well as Plot Renderer activities) can be shown in the Results window as different tabs.

You can only successfully tabulate the results of a single-equilibrium calculation or a stepping operation. The tabulated data from an equilibrium calculation is different from the tabulated data from a stepping calculation.

Also see *Creating Activities and Successors* on page 30 for a list of possible successors and predecessors for this activity.

Tabulated Results from an Equilibrium Calculation

The following tab shows the result of an equilibrium calculation (from example 1 in *Graphical Mode Example Collection* on page 9).



System		
Moles	1.00000	
Mass	55.64392	[g]
Temperature	1000.00000	[K]
Total Gibbs Energy	-42140.55264	[J]
Enthalpy	24707.16903	[J]
Volume	7.29746E-6	[m3]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Fe	0.99537	0.99900	0.00619	-42277.77189
C	0.00463	0.00100	0.21818	-12658.35450

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.99609	55.59691	0.99711	Composition and constitution ▼

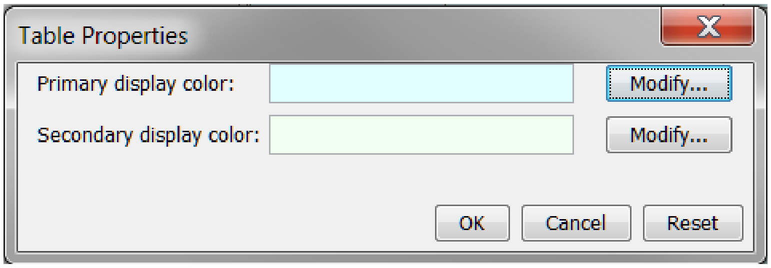
Composition		
Component	*Mole Fraction*	*Mass Fraction*
Fe	0.99928	0.99984
C	0.00072	0.00016

Constitution	$(Fe)_1 (C,VA)_3$	
	Constituent	*Site Fraction*
Sublattice 1:		
	Fe	1.00000
Sublattice 2:		
	VA	0.99976
	C	0.00024

For each stable phase listed, from the **Composition and constitution** menu you can select the information to view. In this example, the maximum amount of information is shown and includes details about both composition and constitution for **BCC_A2#1**.

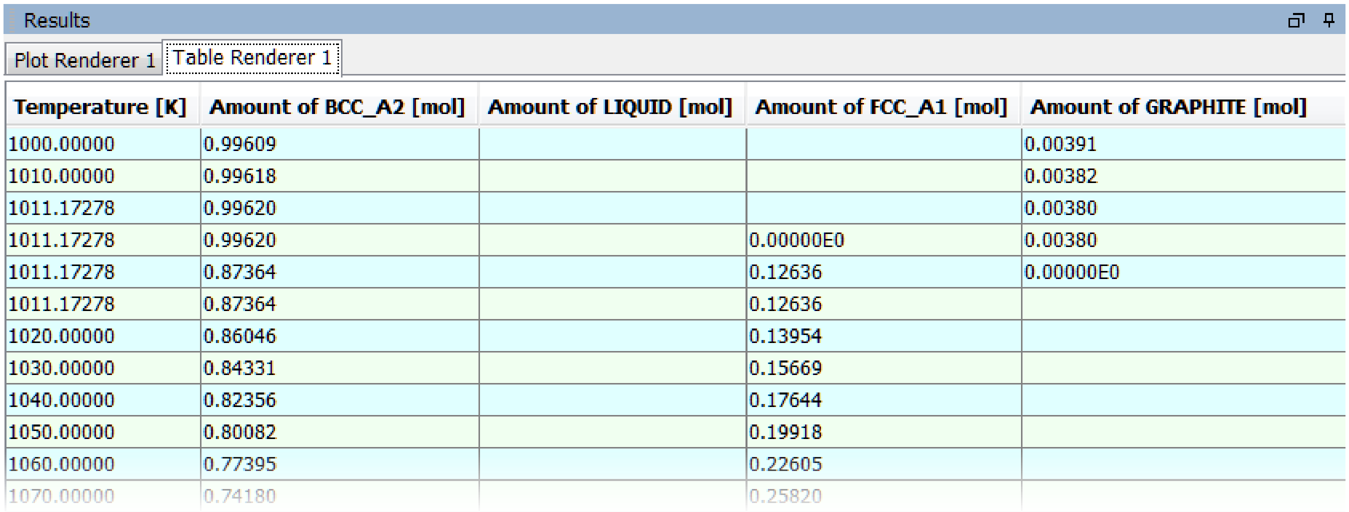
Setting Background Colours

To change the background colours of the table, in the **Results** window right-click a Table Renderer tab, and select **Properties**. Modify as required.



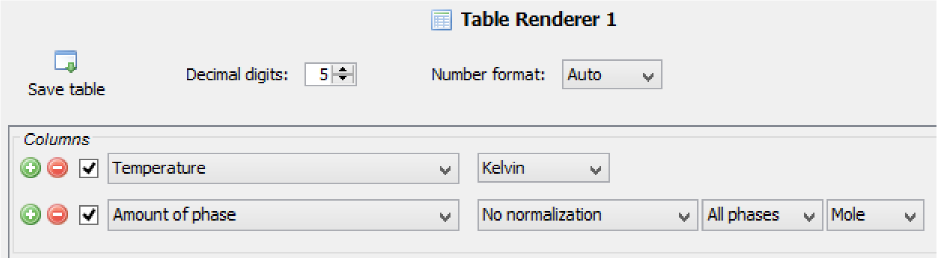
Tabulated Results from a Stepping Operation

The **Table Render 1** tab in the example shows the results of a stepping calculation (from example 2 in *Graphical Mode Example Collection* on page 9).



Temperature [K]	Amount of BCC_A2 [mol]	Amount of LIQUID [mol]	Amount of FCC_A1 [mol]	Amount of GRAPHITE [mol]
1000.00000	0.99609			0.00391
1010.00000	0.99618			0.00382
1011.17278	0.99620			0.00380
1011.17278	0.99620		0.00000E0	0.00380
1011.17278	0.87364		0.12636	0.00000E0
1011.17278	0.87364		0.12636	
1020.00000	0.86046		0.13954	
1030.00000	0.84331		0.15669	
1040.00000	0.82356		0.17644	
1050.00000	0.80082		0.19918	
1060.00000	0.77395		0.22605	
1070.00000	0.74180		0.25820	

Configuration Window Settings



Decimal digits: 5

Number format: Auto

☑ Temperature — Kelvin

☑ Amount of phase — No normalization — All phases — Mole

Defining the Table Columns

In the **Configuration** window for the Table Renderer 1 node, set the level of detail for the Columns:

Setting Number Format and Number of Decimal Digits

The table results can be presented in ordinary decimal number format or with normalized scientific notion. The **Number format** menu defaults to **Auto** to use the most appropriate format based on the tabulated data. Or choose **Scientific** or **Decimal** to increase or decrease the number of **Decimal digits** used in the table.

Saving Tabulated Data

To save all the data in a table as a plain text file, in the **Configuration** window click **Save table** or in the **Results** window right-click in the table and select Save As.

To copy the data from a single cell of a table to the clipboard, right-click the cell and select **Copy**. To copy the whole table to the clipboard, select **Copy all**.

The data saved is what is shown in the **Table Renderer** tab. If data is calculated but not displayed it is not saved.

Experimental File Reader

The Experimental File Reader activity can only be created from the top My Project node. This activity allows you to read an experimental data file (*.EXP). This type of file has information specifying a plotted diagram, written in the DATAPLOT graphical language.

Also see *Creating Activities and Successors* on page 30 and the *DATPLOT User Guide* included with this documentation set.

How to Plot an Experimental Data File

1. Right-click **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
2. In the **Configuration** window in the **EXP file** field, enter the name of the EXP-file to plot.
3. Click **Create New Successor** and select **Plot Renderer**. Or right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.
4. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

Binary Calculator

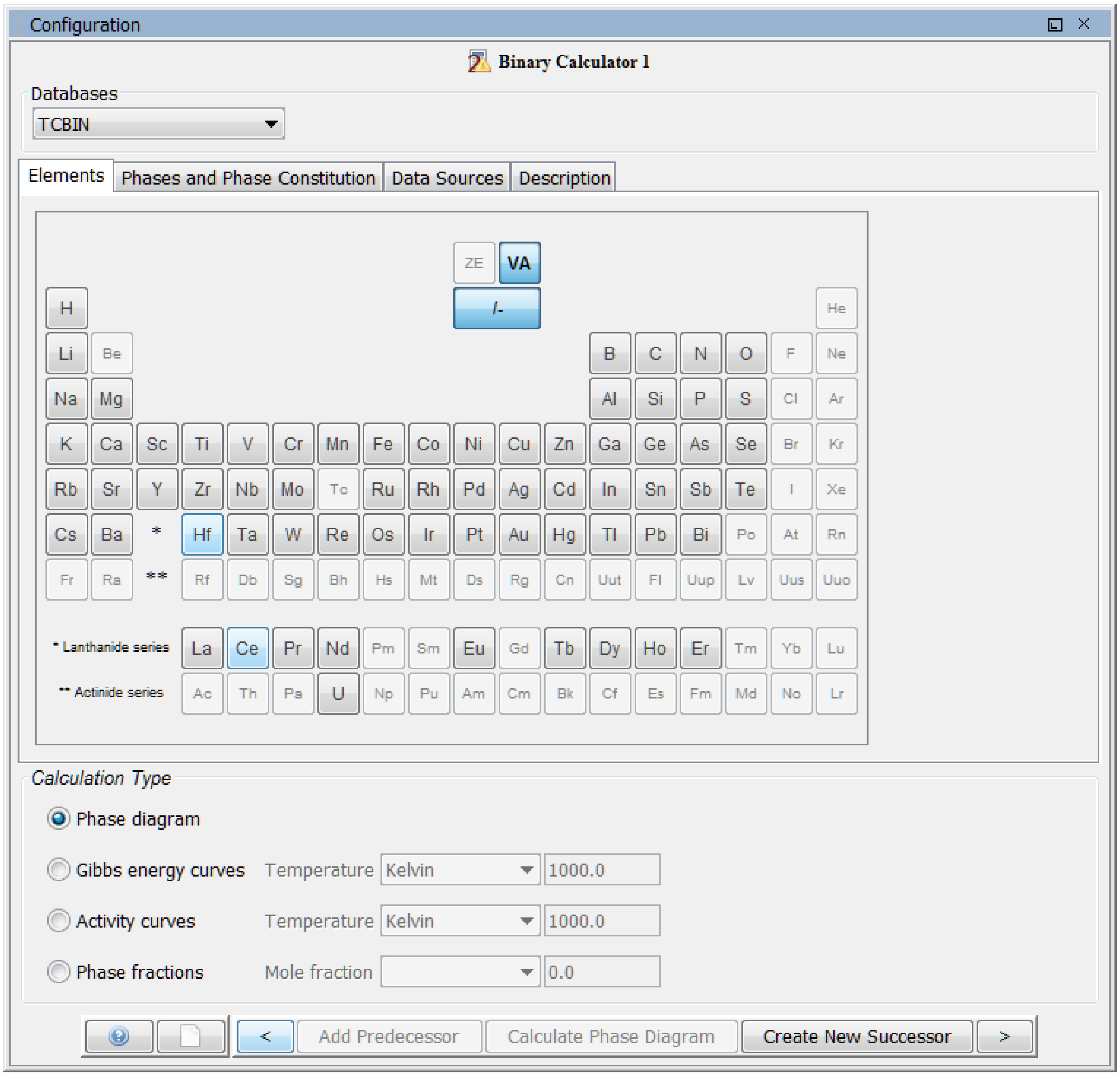
A Binary Calculator can be used for some calculations involving two components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on binary systems.

The Binary Calculator relies on some specifications that are not supported by all databases. You need a specially designed database for the Binary Calculator such as the TCBIN database.

For an example of how a Binary Calculator can be used in a project, see example 3 in *Graphical Mode Example Collection* on page 9.

Configuration Window

The following shows the **Configuration** window of a **Binary Calculator** activity.



Databases: TCBIN

Calculation Type

● Phase diagram

○ Gibbs energy curves   Temperature Kelvin 1000.0

○ Activity curves   Temperature Kelvin 1000.0

○ Phase fractions   Mole fraction 0.0

Configuration Settings

The table lists the available settings to configure before performing the calculation.

Also see *Creating Activities and Successors* on page 30 for a list of possible successors and predecessors for this activity.

Setting	Description
Select database	Select a database that contains specifications dedicated to the Binary Calculator.
Elements (periodic table)	In the periodic table, select the two elements that make up the components of the system.
Phases and Phase Constitution	This tab is the same as for a *System Definer* on page 55. See *Phases and Phase Constitution* for an example.
Data Sources	This tab is the same as for a *System Definer* on page 55. See *Data Sources* for an example.
Description	This tab is the same as for a *System Definer* on page 55. See *Description* for an example.
Calculation Type	
Phase diagram	Select to perform a mapping calculation. Click **Calculate Phase Diagram** to plot the results.
Gibbs energy curves	Select the **Temperature** and click **Calculate Gibbs Energy Curves** to calculate at a constant temperature over the whole composition range.
Activity curves	Select the **Temperature** and click **Calculate Activity Curves** to calculate at a constant temperature over the whole composition range.
Phase fractions	Select the **Mole fraction** and click **Calculate Phase Fractions** to calculate as a function of temperature at a constant composition.

Ternary Calculator

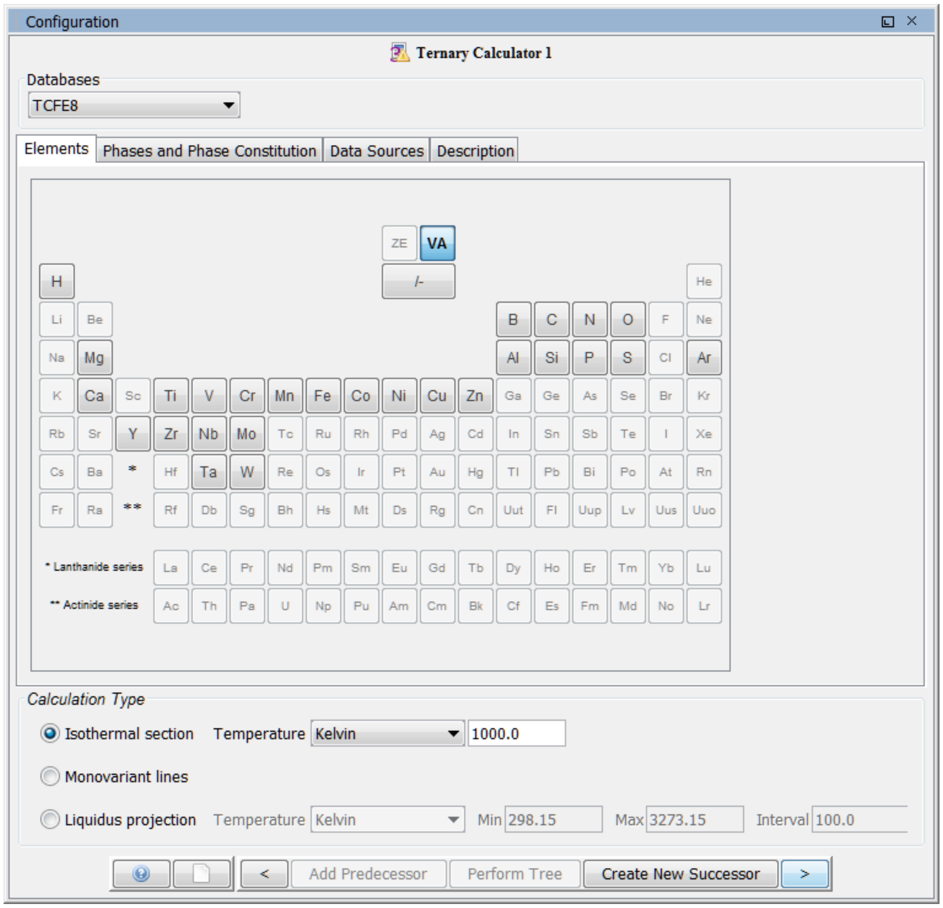
A Ternary Calculator is used for some calculations involving three components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on ternary systems.

For an example of how a Ternary Calculator is used in a project, see example 4 in *Graphical Mode Example Collection* on page 9.

Also see *Creating Activities and Successors* on page 30 for a list of possible successors and predecessors for this activity.

Configuration Window

The following shows the Configuration window of a Ternary Calculator activity:



Databases: TCFE8

● Isothermal section Temperature Kelvin 1000.0

○ Monovariant lines

○ Liquidus projection Temperature Kelvin Min 298.15 Max 3273.15 Interval 100.0

Configuration Settings

The table lists the available settings that must be configured before performing the calculation.

Setting	Description
Select database	Select a database that contains specifications dedicated to the Ternary Calculator.
Elements (periodic table)	In the periodic table, select the three elements that make up the components of the system.

Setting	Description
Phases and Phase Constitution	This tab is the same as for a *System Definer* on page 55. See *Phases and Phase Constitution* for an example.
Data Sources	This tab is the same as for a *System Definer* on page 55. See *Data Sources* for an example.
Description	This tab is the same as for a *System Definer* on page 55. See *Description* for an example.
Calculation Types	
Isothermal section	Select the **Temperature** at which the ternary system is calculated for the whole composition range.
Monovariant lines	The variation of the liquid compositions with temperature is calculated.
Liquidus projection	Select the **Temperature** range (**Min** and **Max**) and an **Interval**. The projection liquid surface and the monovariant lines are calculated over the given temperature range.

Scheil Calculator

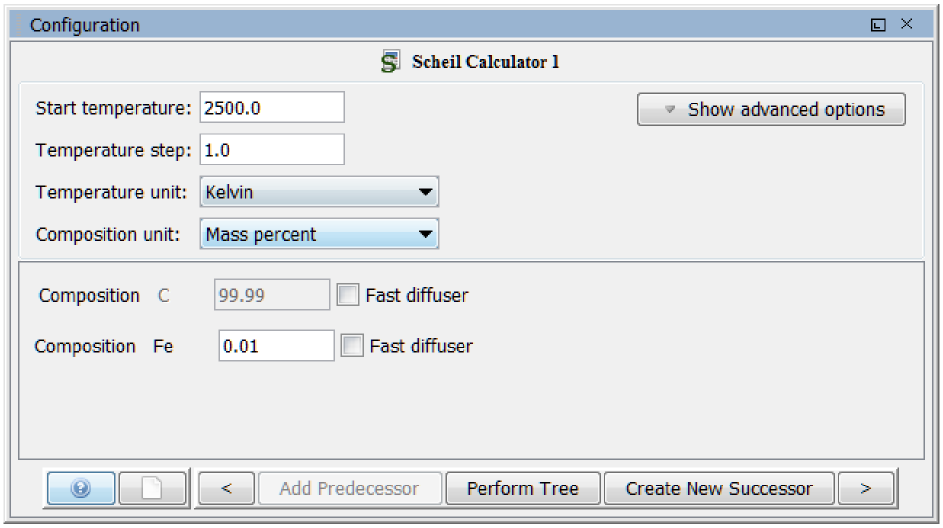
The Scheil Calculator activity is used to perform simulations of *Scheil (Scheil-Gulliver) solidification processes*. By default, a Scheil calculation results in an estimation of the solidification range of an alloy. The calculation is based on the assumption that the liquid phase is homogeneous at all times and that the diffusivity is zero in the solid. However, it is possible to disregard the latter assumption for selected components.

By default, a Plot Renderer successor has the default plot axes **Mole fraction of solid** (X-axis) and **Temperature Celsius** (Y-axis). When these default axes are used in the Plot Renderer, the results of normal equilibria calculations are automatically plotted in the same diagram as the Scheil calculations.

See example 8 in *Graphical Mode Example Collection* on page 9.

Configuration Window

The main **Configuration** window of a **Scheil Calculator** activity is shown below and listed in the table. These settings must be configured before performing the calculation.



Start temperature: 2500.0

Temperature step: 1.0

Temperature unit: Kelvin

Composition unit: Mass percent

Composition C 99.99 ☐ Fast diffuser

Composition Fe 0.01 ☐ Fast diffuser

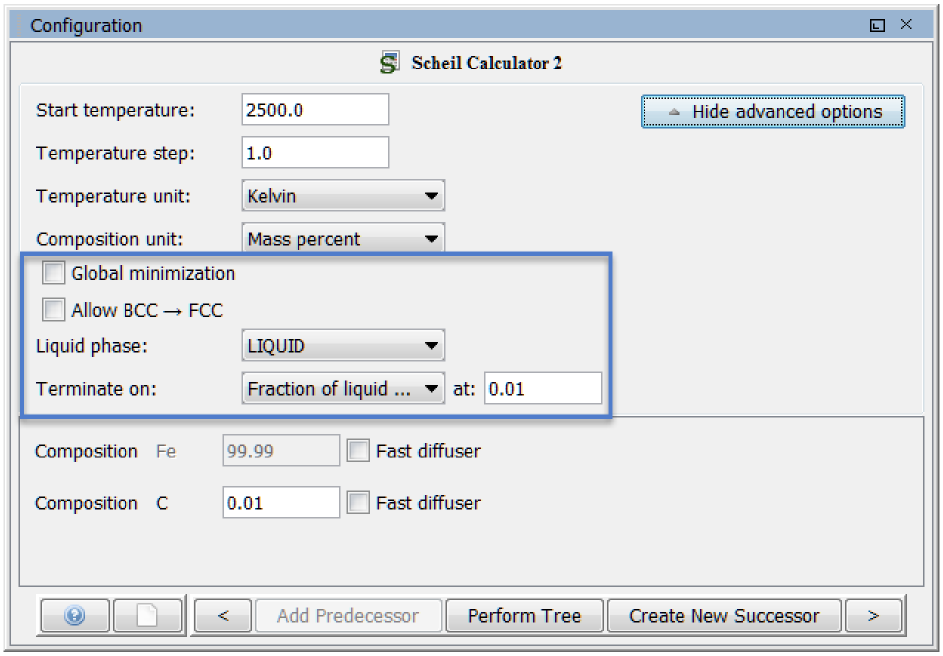
Configuration Settings

Setting	Description
Start temperature	Enter a **Start temperature** that is higher than the liquidus temperature of the alloy, in other words, the temperature at which the alloy is completely melted.
Temperature step	Enter a **Temperature step**. Decreasing the temperature step increases the accuracy, but the default value is usually adequate.
Temperature unit	Select the **Temperature unit**: **Kelvin**, **Celsius** or **Fahrenheit**.
Composition unit	Select the **Composition unit**: **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.
Composition	This is based on what is entered in the *System Definer* on page 55.
Fast diffuser	Click to select the **Fast diffuser** check box to allow redistribution of this component in both the solid and liquid parts of the alloy.

Scheil Calculator Advanced Options and Settings

Additional advanced settings are available as shown below and in the table:

Click **Show advanced options** to open this configuration window:



Configuration

Scheil Calculator 2

Start temperature: 2500.0
Temperature step: 1.0
Temperature unit: Kelvin
Composition unit: Mass percent
☐ Global minimization
☐ Allow BCC → FCC
Liquid phase: LIQUID
Terminate on: Fraction of liquid ... at: 0.01
Composition Fe 99.99 ☐ Fast diffuser
Composition C 0.01 ☐ Fast diffuser

Scheil Calculator Advanced Settings

Setting	Description
Global minimization	By default the **Global minimization** check box is not selected. Click to select it to perform a global minimization test when an equilibrium is reached. This costs more computer time but the calculations are more robust.
Allow BCC→FCC	By default the **Allow BCC → FCC** check box is not selected. Select the check box to allow transformations in the solidified part of the alloy caused by each of the components specified to be a *fast diffuser*. It is recommended that you only select this for steels.
Liquid phase	The default in the list is the **Liquid phase** already defined in the database.
Terminate on	Enter a value to terminate the calculation on the **Fraction of liquid phase** or at a specific **Temperature**.
Max no. of iterations	By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
Required accuracy	The default is 1.0E-6. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Setting	**Description**
Smallest fraction	The default is 1.0E-12. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30. In Console Mode, the default of 1E-30 is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system.
Approximate driving force for metastable phases	The check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favourable composition and thus their driving forces may be only approximate. If it is important that these driving forces are correct, click to clear the check box to force the calculation to converge for the metastable phases.

Also see *Creating Activities and Successors* on page 30 for a list of possible successors and predecessors for this activity and *Scheil Simulations* on page 146 in the Console Mode section.

The Console Mode Interface

The following is an introduction to the Console Mode’s user interface and the command line prompt.

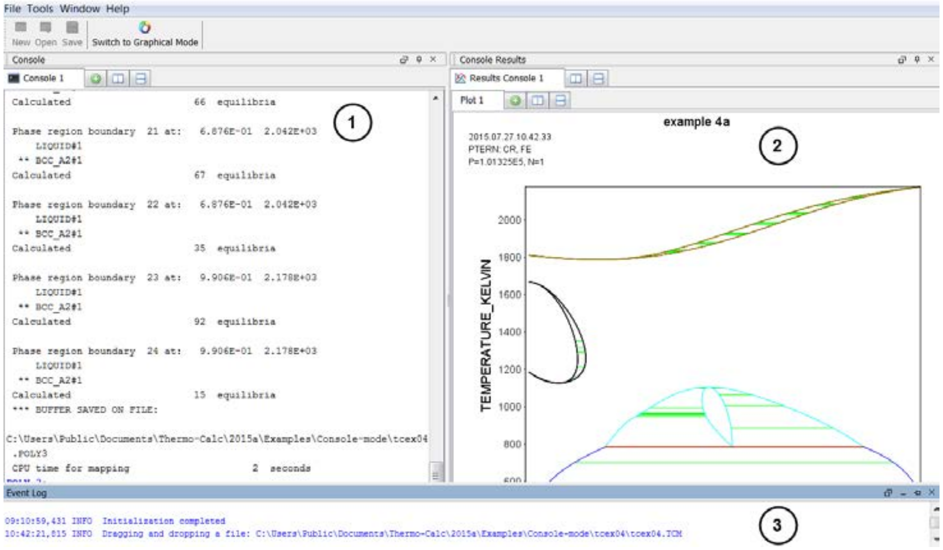
Also see *The Graphical Mode Interface* on page 27 for information about that mode.

In this section:

The Console Mode Layout

By default the first time you launch Thermo-Calc it opens in Graphical Mode. After this, the mode defaults to the most recent one. You can switch back and forth between modes. To open the Console Mode interface, click **Switch to Console Mode** on the toolbar.

The Console Mode User Interface



```
Calculated                     66  equilibria

Phase region boundary  21 at:   6.876E-01  2.042E+03
    LIQUID#1
 ** BCC_A2#1
Calculated                     67  equilibria

Phase region boundary  22 at:   6.876E-01  2.042E+03
    LIQUID#1
 ** BCC_A2#1
Calculated                     35  equilibria

Phase region boundary  23 at:   9.906E-01  2.178E+03
    LIQUID#1
 ** BCC_A2#1
Calculated                     92  equilibria

Phase region boundary  24 at:   9.906E-01  2.178E+03
    LIQUID#1
 ** BCC_A2#1
Calculated                     15  equilibria
 *** BUFFER SAVED ON FILE:

C:\Users\Public\Documents\Thermo-Calc\2015a\Examples\Console-mode\tcex04
 .POLY3
 CPU time for mapping                       2  seconds
```

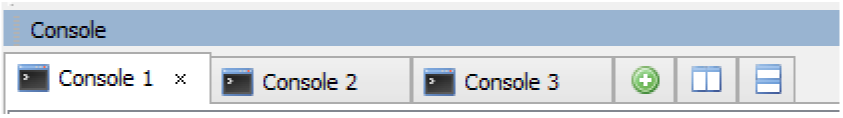
```
09:10:59,431 INFO  Initialization completed
10:42:21,815 INFO  Dragging and dropping a file: C:\Users\Public\Documents\Thermo-Calc\2015a\Examples\Console-mode\tcex04\tcex04.TCM
```

The currently selected window is called the *active* window. This has a darker title bar than the other windows. The windows are:

1. **Console**, with a **Console 1** tab.
2. **Console Results**, with a **Results Console 1** tab as well as a sub-tab (**Plot 1**), which is what is displayed in the window in the figure.
3. **Event Log**, which is the active window in this example.

Console Tabs

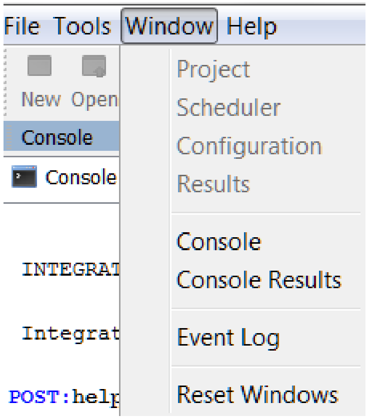
By default, the tabs are side-by-side:



You can toggle to view the tabs top-to-bottom/stacked (click the ⊟ button) and back to side-by-side (click the ◫ button) or the ▭ button.

Open Console Windows

Open a specific window from the **Window** main menu, or select **Reset Windows** to return to the default window layout.



Console Window

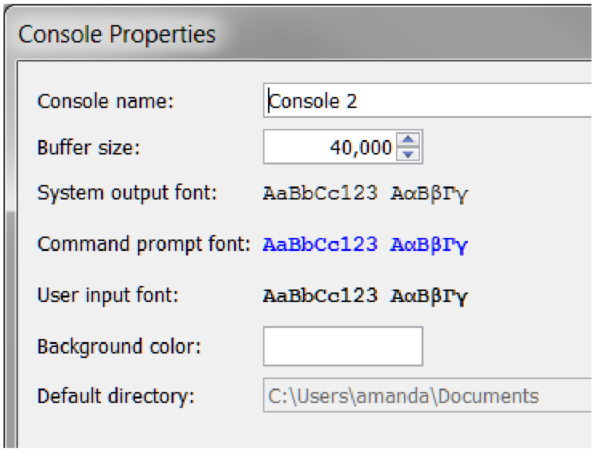
By default the Console window is on the left-hand side of the console. This is where you enter commands. The window can have several Console tabs.

To open and close Console tabs:

- To open (or add), click the ⊕ button, press <Ctrl+T> when the Console window is active, or right-click a tab header and select **New Console**.
- To close, click the ⊖ button, press <Ctrl+W> or <Ctrl+F4>, or right-click the tab header and select **Close**.
- To close all tabs except one, right-click the header of the tab you want to keep and select **Close Other**.
- To close all tabs and open a new one, right-click the header of any tab and select **Close All**.

You can change the tab name, font and colours for an individual Console tab by right-clicking its header and selecting **Properties**.

Console Properties Window



Console Properties

Console name: Console 2
Buffer size: 40,000
System output font: AaBbCc123 AαBβΓγ
Command prompt font: AaBbCc123 AαBβΓγ
User input font: AaBbCc123 AαBβΓγ
Background color:
Default directory: C:\Users\amanda\Documents

Editing the Default Console Directory

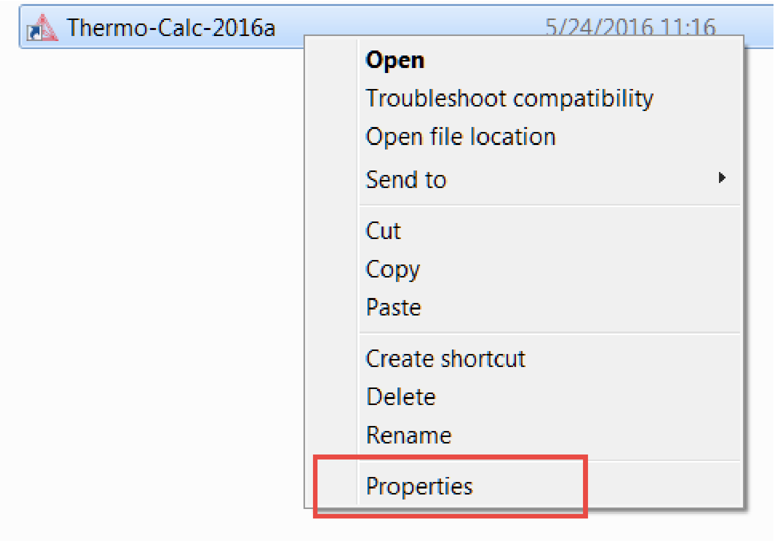
You can add a startup parameter to a shortcut when launching Thermo-Calc on any of the platforms. When you launch the revised shortcut, the file path is set to a user-defined default directory. An example of why you might want to have a custom directory path is if you use batch projects or if you have macro files for batch jobs. The custom directory file path can also be viewed from within Console Mode.

> The shortcut is only valid throughout the existing session; it is not saved as a default. Each time you want to use this file path you must launch Thermo-Calc from the customized shortcut.

The following uses Windows for the example.

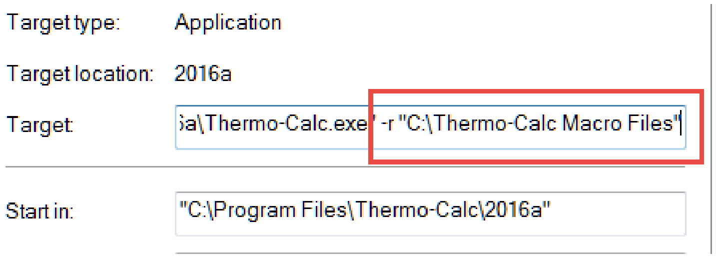
Setting up the Default Console Directory

1. Right-click a shortcut to Thermo-Calc and click **Properties**.



2. In the **Thermo-Calc 2016a Properties** dialog, **Target** field, add the following to the end of the string: **–r** plus the *“path to the default directory”*. Include a space between the –r and path, and use quotation marks around the full file path. A simple example:

   -r “C:\Thermo-Calc_Macro_Files”

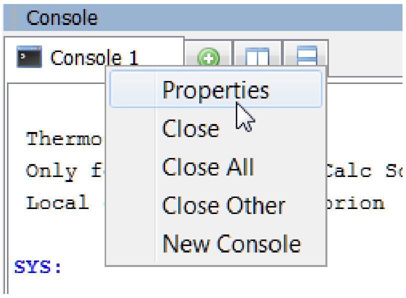


Target type: Application
Target location: 2016a
Target: a\Thermo-Calc.exe" -r "C:\Thermo-Calc Macro Files"
Start in: "C:\Program Files\Thermo-Calc\2016a"

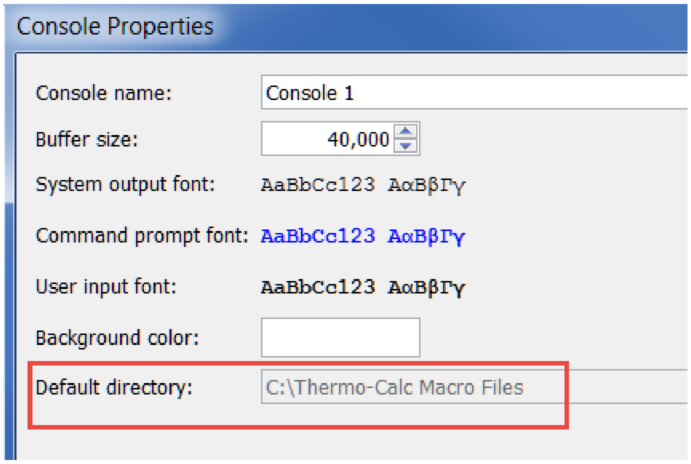
3. Click **Apply** and **OK**.
4. Launch Thermo-Calc from the shortcut where you added the parameter. You can confirm that it is set correctly from within Thermo-Calc.

Viewing the File Path in Thermo-Calc

1. Launch Thermo-Calc from the short cut where you added the parameter.
2. In Console Mode, right click the **Console** window and choose **Properties**.



3. In the **Console Properties** window the **Default directory** section displays the custom file path.



Console Properties

Console name: Console 1
Buffer size: 40,000
System output font: AaBbCc123 AαBβΓγ
Command prompt font: AaBbCc123 AαBβΓγ
User input font: AaBbCc123 AαBβΓγ
Background color:
Default directory: C:\Thermo-Calc Macro Files

Console Mode Results Window

By default, the Console Results window is on the right-hand side of the screen. This is where plotted diagrams display. Each Console has its own Results tab in the Results window. All the plots and tables generated are presented in the Results tab.

- To open new **Plot** tabs press <Ctrl+Shift+T> or click the add ⊕ button.
- To open a new Plot tab for the currently active Console tab, press <Ctrl+Shift+T>. To close the Plot tab, press <Ctrl+Shift+W> or <Ctrl+Shift+F4>.

Event Log Window

By default the Event Log window is collapsed (closed). It includes important information about the commands that run and are completed, including error messages. Click once to toggle it open and closed.

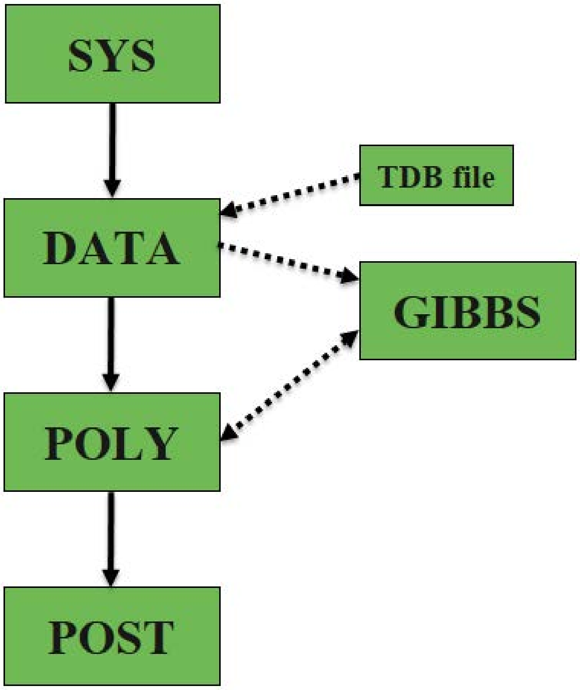
Console Mode Workflow

Working with Thermo-Calc involves moving between different modules. The workflow differs depending on the type of calculation:

- If you want to perform a calculation using the POLY module, you typically first retrieve thermodynamic data in the DATA module, perform the calculation in POLY, and visualize the results in the POST module. It is possible to define a system directly in POLY using *DEFINE_MATERIAL* on page 147 and *DEFINE_DIAGRAM* on page 144.
- If you want to calculate and plot a diagram using a response-driven module, such as POTENTIAL or SCHEIL, then you can go directly to that module. Response-driven modules prompt you to go through the steps to do the calculation and the required post-processing. These modules include BIN, TERN, POTENTIAL, POURBAIX, and SCHEIL. You typically end up in the POST module after having used a response-driven module. In the POST module you can modify the plots and save the diagram.
- If you want to tabulate a chemical substance, phase, or reaction, go directly to the TAB module.

Typical POLY Module Workflow

The following represents the typical workflow when you perform calculations in the POLY module. The solid arrows represent your typical movements between the modules. The dashed arrows represent the movement of data within Thermo-Calc.



The basic workflow is:

1. You are in the **SYS** module when you start Thermo-Calc in Console Mode.
2. In the **DATA** module define the system. Before performing a calculation, you must define the system and retrieve thermodynamic data. The data is retrieved from a database file (*.TDB or *.TDC).
3. The data needed to describe a system is then sent to the **GIBBS** module. This data is accessed by the **POLY** module when you instruct it to perform calculations.
4. In the **POLY** module, perform the calculations.

- In POLY, the conditions are set for an equilibrium calculation (temperature, pressure, system composition, etc.), then an equilibrium calculation is done.
- If you want to make a property or phase diagram, you set the conditions for a stepping or mapping operation and perform that operation.
- This generates data that can be used to plot a property diagram (if a stepping operation is performed) or a phase diagram (if a mapping operation is performed).

5. In the **POST** module plot and visualize your data.

- If a stepping or mapping operation is performed, then you can go to the POST module and plot a property or phase diagram.
- The diagram can be plotted quickly using default settings, but you can also modify which variables to plot of the diagram axes and change the appearance of the diagram.
- You can save the diagram either as a plain text file with data about all the coordinates or as an image file.

Performing Calculations in Console Mode

Calculations can be performed either in the POLY module, or using some of the response-driven modules designed to perform specific types of calculations.

About Equilibrium Calculations on page 133 describes generally how to calculate and plot *Property Diagrams* and *Phase Diagrams*. To calculate and plot a property diagram or a phase diagram, you must first calculate an equilibrium.

Additional sections of use include *About Scheil Simulations* on page 147, *T0 Temperature Simulations* on page 153, *About Paraequilibrium* on page 156, *About Potential Diagrams* on page 160, and *About Aqueous Solutions* on page 164. Also search the online help or see *TABULATION_REACTION Commands* on page 247 and *POLY_3 Commands* on page 117 in the *Thermo-Calc Console Mode Command Reference*.

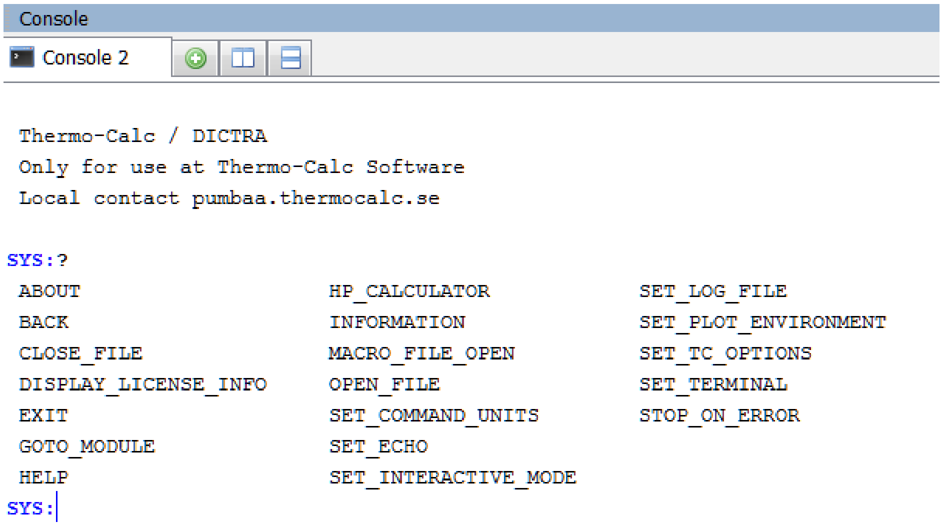
Using the Command Line Prompt

The command line prompt in the Console window tells you which module you are currently in. When Thermo-Calc is first opened in Console Mode, you are in the SYS module, which is indicated with the command line prompt `SYS`.

To use Console Mode, you type in commands at the command line prompt. The available commands depend on which module you are in. You can list the commands by typing `?` at the prompt and then press <Enter>.

- *Moving Between Modules and Submodules* below
- *Entering Command Names or Abbreviations* on the next page
- *Specifying Parameters* on page 123
- *Wild Card Characters* on page 124
- *Controlling Console Output* on page 125
- *Command History* on page 125

Available SYS Module Commands



```
Thermo-Calc / DICTRA
Only for use at Thermo-Calc Software
Local contact pumbaa.thermocalc.se

SYS:?
 ABOUT                   HP_CALCULATOR           SET_LOG_FILE
 BACK                    INFORMATION             SET_PLOT_ENVIRONMENT
 CLOSE_FILE              MACRO_FILE_OPEN         SET_TC_OPTIONS
 DISPLAY_LICENSE_INFO    OPEN_FILE               SET_TERMINAL
 EXIT                    SET_COMMAND_UNITS       STOP_ON_ERROR
 GOTO_MODULE             SET_ECHO
 HELP                    SET_INTERACTIVE_MODE
SYS:
```

Moving Between Modules and Submodules

To go to a specific module, you typically use GOTO_MODULE (or just GOTO) followed by the name of the module. For example, to go to the DATA module, type `GOTO DATA`.

The exceptions are the submodules POST and ED-EXP:

- To go to the POST module, you must enter the POST command from within the POLY module or DICTRA module (if you have the add-on license).

- To go to *Experimental Data Files* on page 36, you must enter the ED-EXP command from within the PARROT module.

To go back to the previous module type `Back`. For example, if you are in the DATA module and entered it from the SYS module, when you type `Back`, you return to the SYS prompt. This command is also available to exit from the submodules POST and ED-EXP.

Without a valid Thermo-Calc license, you cannot leave the SYS module. To enter the DICTRA and DIC_PARROT modules, you also need a valid Diffusion Module (DICTRA) license key.

Entering Command Names or Abbreviations

The name of a command typically consists of terms linked with underscores, for example, *LIST_EQUILIBRIUM* on page 156. Note the following:

- UPPER or lower case letters are OK.
- Hyphens (-) instead of underscores (_) are OK, e.g. LIST-EQUILIBRIUM.
- You can abbreviate commands as long as it is unambiguous, e.g. when more than one command begins with LIST_, you need to type the next letter or word to distinguish between the commands.
- Each word can be abbreviated e.g., L_E for LIST_EQUILIBRIUM.

Command Names and Abbreviations Examples

These are examples of how you can abbreviate commands at the command line prompt.

Command name	Abbreviation
CALCULATE_EQUILIBRIUM	C-E
CALCULATE_ALL_EQUILIBRIA	C-A
LIST_EQUILIBRIUM	L-E
LIST_INITIAL_EQUILBRIUM	LI-I-E
LOAD_INITIAL_EQUILBRIUM	LO-I-E
LIST_PHASE_DATA CBCC	L-P-D CBC
LIST_PHASE_DATA CEMENTITE	L-P-D CEM
SET_ALL_START_VALUES	S-A-SS-AL
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025	S-A-V 1 X(F,FE) 0 .89 .025

Command name	Abbreviation
SET_START_CONSTITUENT	S-S-C
SET_START_VALUE	S-S-V
SET_AXIS_PLOT_STATUS	S-A-P
SET_AXIS_TEXT_STATUS	S-A-T-SS-A-TE
SET_AXIS_TYPE	S-A-TY
SET_OPTIMIZING_CONDITION	S-O-C
SET_OPTIMIZING_VARIABLE	S-O-V
SET_OUTPUT_LEVEL	S-O-LS-OU

Specifying Parameters

Running a command typically requires that several parameter values are specified, which can be done directly in the command line after the command name. For example, to set an axis variable for a stepping or mapping operation, enter:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

You can also use SET_AXIS_VARIABLE and press <Enter>. At the command line prompt, you then specify the parameters one at a time.

On all command lines, you can enter a question mark (`?`) for help. For some parameters, enter two question marks (`??`) for more detailed information.

Default Parameters Values

When you are requested to specify a parameter, Thermo-Calc usually suggests an appropriate default value, which is displayed at the prompt between two slash signs (//). For example, this prompt means the default answer is `TERMINAL`:

```
OUTPUT FILE /TERMINAL/:
```

Press <Enter> to accept the default.

If you specify some parameters directly after the command name, then you can still choose to accept default values for some parameters.

To accept the default value for a parameter, type a comma (,) instead of a value for that parameter. For the comma to be interpreted correctly, type a blank space on each side of the comma. However, if you accept the default values for several parameters that follow each other, then the commas can be typed in without blank spaces separating them: (, , ,) is interpreted in the same way as (,   ,   ,).

For some commands and parameters, Thermo-Calc treats the values previously assigned as default values if the command is used again. For example, if the first stepping or mapping axis variable is specified as:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

Then if you want to change a parameter value for this axis variable, type:

```
SET_AXIS_VARIABLE 1 , 0.1 ,,,
```

This changes the minimum value from 0 to 0.1 at which a stepping or mapping operation halts. The other parameter values remain the same. Consequently, what is typed is equivalent to:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0.1 0.89 0.025
```

Wild Card Characters

You can sometimes use the asterisk (`*`) as a wild card character to, for example, refer to all components, phases, or species, when showing calculated properties in the POLY module, or when you set axis variables for plotting diagrams in the POST module.

When showing calculated properties in the POLY module, you can also use the dollar sign (`$`) to refer to all stable phases.

For activity and/or chemical potential properties, the `*`and `$` normally do not work properly as wild card characters.

Wild Card Character Examples

These are examples of the wild card characters you can use to search commands at the command line prompt.

Command	Action
SHOW_VALUE B(*)	Lists mass (gram) of all components in the system.
SET_AXIS_VAR Y B(*) *	Sets mass (gram) of all components in the system as Y-axis variable.
SHOW_VALUE MUR(*)	Lists chemical potentials of all components in the system.
SET_AXIS_VAR Y ACR(*) *	Sets activities of all components in the system as Y-axis variable.
SHOW_VALUE HM(*).T	Lists heat capacities of all phases.
SET_AXIS_VAR Y GM(*) *	Sets molar Gibbs free energies of all phases as Y-axis variable.
SHOW_VALUE TC($)	Lists curie temperature of all stable phases.
SHOW_VALUE W(*,*)	Lists mass fractions of all components in all phases.
SHOW_VALUE W($,*)	Lists mass fractions of all components in all stable phases.

Command	Action
SHOW_VALUE W(FCC,*)	Lists mass fractions of all components in the FCC phase.
SHOW_VALUE W(*,FE)	Lists mass fractions of the Fe component in all phases.
SHOW_VALUE W($,FE)	Lists mass fractions of the Fe component in all stable phases.
SHOW_VALUE Y(*,*)	Lists site fractions of all species in all sublattices of all phases.
SHOW_VALUE Y($,*)	Lists site fractions of all species in all sublattices of all stable phases.
SHOW_VALUE Y(*,*)	Lists site fractions of all species in all sublattices of all phases.

Controlling Console Output

In response to a command Thermo-Calc may display a lot of text in the Console window.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a mapping operation, the results are continuously printed in the Console window. To terminate the calculation of the current region of the mapping and stop the output, press <Ctrl+C>.

Command History

- To scroll through the last twenty commands used, type two exclamation marks (`!!`) and press <Enter>.
- To repeat the last n commands, type `!` followed by the number of previous commands to be executed again.
- To scroll through previous performed commands, use the Up (↑) or Down arrow (↓) keys.
- To read more information about the command history functionality in Thermo-Calc, type `! ?` at the command line prompt.

Log, Macro and Workspace Files

In Console Mode, Thermo-Calc uses different kinds of files, including:

- *Log Files* on the next page (*.LOG)
- *Macro Files* on the next page (*.TCM or *.LOG)

- POLY *Workspace Files* on page 128 (*.POLY3),
- *Experimental Data Files* on page 36 (*.EXP)

Also see the *Data Optimization User Guide* on page 1.

- The GIBBS module uses a workspace file (*.GES5). See *GIBBS_ENERGY_SYSTEM Commands* on page 42
- The PARROT module uses files with the suffixes *.PAR and *.POP. See *PARROT Commands* on page 86

Log Files

Log files are plain text files used to save a sequence of commands. Log files can be edited in a text editor.

- To start saving your input into such a file, use SET_LOG_FILE in the SYS module, followed by the name of the file that you want to save your command sequence to.
- If you want to save the output in the log file as well, use SET_ECHO before the SET_LOG_FILE command. Doing this is useful if you want use the log file later as a macro file.

See *SYSTEM_UTILITIES Commands* on page 241 in the *Thermo-Calc Console Mode Command Reference*.

Macro Files

Macro files are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor.

Macro File Commands

Also see Example 12 in *Console Mode Example Collection* on page 14.

Action	**Command**	**Description and Comments**
To load a macro file	In the SYS module, *MACRO_FILE_OPEN* on page 5 followed by the name of the macro file.	Thermo-Calc starts the command sequence that the file contains.
Regain control of the console	*SET_INTERACTIVE* on page 237	End a macro file with this command to have control of the Console returned to you.

Action	Command	Description and Comments
Add comments to a macro file	Start a line with @@, or enclose it between an @ (-line and a @)-line.	When lines are enclosed the software ignores them when running the macro.
Open a macro file	MACRO_FILE_OPEN	When creating the log file, you can make a macro file load up to five other macro files.
Nest macro files inside of each other	MACRO_FILE_OPEN SET_INTERACTIVE	If a nested macro file ends with SET_INTERACTIVE, then Thermo-Calc resumes with the higher-level macro file at the command immediately following the MACRO_FILE_OPEN command that loaded and executed macro file that has just been terminated. If a nested macro file doesn’t end with SET_INTERACTIVE (but with an end-of-file character), then the console shuts down and the macro is stopped.

Macro File Control Characters

The `@?` character allows you to make a macro interactive by allowing input. At the @? character, which is placed where a parameter value or argument is normally put, Thermo-Calc prompts to input the value of a parameter or argument. You can enter a string immediately following the @? character. This string is presented to the user when prompted to enter the parameter value or argument. The entered value is used by Thermo-Calc as input to the command in question. For example, you can request the user to specify the temperature range of a stepping calculation by entering the following in a macro file:

```
SET_AXIS_VARIABLE 1 T @?Low-temperature-limit: @?High-temperature-
limit:
```

You can also use up to nine variables in your macro file and prompt the user to enter values that can be assigned to these variables. Use the `@#n` character when you want to prompt the user to provide a value to the variable, where the n is a digit between `1` and `9`. You can then use this value by with the `##n` character. For example, you can request the user to provide the first element of a system by entering the following in the macro file:

```
@#3First-element?
```

You can then use this variable with the entering the character ##3 later in the macro file. For example, you can write:

```
SET_AXIS_VARIABLE 1 x(##3) 0 1,,,
```

Finally, there is the `@&` pause character. Thermo-Calc pauses and waits for input from the user when this pause character is read from a macro file. Inserting pause characters is useful if you want to allow the user to monitor what is happening when Thermo-Calc is running the macro.

Response-Driven Modules and Macros

Macro files that are created while you use a *response-driven module* begin with the module-entering command (for example, `Goto_Module Scheil)` followed by a number of lines with responses to the module's questions and requests. The file terminates with the commands *POST* on page 160 or *SET_INTERACTIVE* on page 237 (this command gives you back control of the Console). An empty line cannot be edited with any input rather than the default answer (to a specific question). Comment lines, commands to open other macro files, pause characters or input-controlling characters cannot be inserted between these empty lines (otherwise the response-driven module cannot be executed properly).

Workspace Files

You can save all the data in your current workspace by first using SAVE_WORKSPACES . This command is available in the POLY, GIBBS and PARROT modules. The workspace has all the settings specified and the result of any stepping or mapping operations performed after using SAVE_WORKSPACES. Consequently, the command opens a workspace in which all data is saved which is generated after the SAVE_WORKSPACE command is executed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and calculation results.

To load the data and calculation results of a workspace file, use the READ_WORKSPACES command available in the POLY module. The file can be used for calculation in POLY, visualization in POST, or data manipulation in GIBBS. You are also given the option in the POURBAIX and SCHEIL modules to open a previously saved workspace file. This allows you to make new POURBAIX or SCHEIL calculations on the same chemical system as before but with different temperature, pressure, and composition conditions, or to plot new property diagrams based on the previous calculations.

Main Menu Commands

The **File** menu and toolbar are reserved for Graphical Mode. In Console Mode you use commands to access these menu options. The **Tools**, **Window** and **Help** menus are described in *Main Menu and Toolbar* on page 33. If there is an equivalent command, it is listed in the table below.

Console Mode Main Menu Commands

Option	Command
Open files	In Thermo-Calc, drag and drop the file into the Console window. In the SYS module: *MACRO_FILE_OPEN* on page 5 In the SYS module: *OPEN_FILE* on page 243
Save (workspace)	This command depends on the module you are in. Type ? at the prompt to look for a command such as *SAVE_GES_WORKSPACE* on page 84 (GIBBS module)
Exit	In any module: EXIT
Close	In the SYS module: *CLOSE_FILE* on page 242
Display license info	In the SYS module: *DISPLAY_LICENSE_INFO* on page 242

Defining a System in Console Mode

Defining a system means to select the chemical components and to retrieve thermodynamic data about those components from an appropriate database in order to do the calculations. You use database(s) with thermodynamic data and then define what system elements as components. Once the system is defined, you retrieve the system’s thermodynamic data from the database(s).

- If you use a *response-driven module* to perform your calculation, such as BIN or POURBAIX, then the module prompts you to select database(s) and define the system.
- When doing calculations in the POLY module, you typically have to manually select databases and define the system in the DATA module. However, it is also possible to define the system directly in POLY using *DEFINE_MATERIAL* on page 147 and *DEFINE_DIAGRAM* on page 144.

Also see *DATABASE_RETRIEVAL Commands* on page 11 in the *Thermo-Calc Console Mode Command Reference*.

How to Define a System in Console Mode

1. Go to the DATA module. At the `SYS` prompt, use GOTO_MODULE and enter `Data`.
2. Change the default database unless you directly specify the name of the database as a parameter to the command. Type `SWITCH_DATABASE` and follow the prompts.

   The second part of the command prompt indicates the current default database. For example, if the prompt is `TDB_TCFE8`, then the current database is TCFE8.

3. Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE and choose `Elements`). For example, if you want to have Fe and C in your system, type:

   ```
   DEFINE_ELEMENTS Fe C
   ```

4. Use REJECT and choose `Phases` if you want to avoid retrieving any phases from the database. (To list the phases that are available in your current database, use LIST_DATABASE and choose `Phases`. To list the phases that can form in the defined system, use LIST_SYSTEM and choose `Constituent`.) For example, if you do not want the graphite phase to be retrieved, you type:

   ```
   REJECT PHASES GRAPHITE
   ```

   If the number of phases to include is much lower than the total number of phases, then it can be convenient to first `Reject Phases *` and then restore the phases to include using `Restore Phases`.

5. Use GET_DATA to search the database and send the thermodynamic data about your system to the GIBBS workspace.

   At this point you can proceed to the POLY module (with GOTO_MODULE POLY). However, you may want to add elements, phases and species to the GIBBS workspace from other databases. If so, then proceed to the next step.

6. Use APPEND_DATABASE to select the (additional) database from which you want to retrieve data. This command works exactly in the same way as the SWITCH_DATABASE command, with the exception that it does not reinitialize the DATA module and the GIBBS workspace, but instead appends or replaces the data that has already been retrieved with new data from the additional database.
7. Define your elements and specify whether to reject and restore any phases. Do this in

exactly the same way when using the SWITCH_DATABASE command (see steps 2 and 3).

8. Use GET_DATA to search the database and add the thermodynamic data to the data that already exists in the GIBBS workspace.
9. Use APPEND_DATABASE again if you want to add data from yet another database. When you have retrieved all the data you need, you can proceed to the POLY module.

Equilibrium Calculations

In this section:

About Equilibrium Calculations

An equilibrium describes what the composition of the end state of a system is, given a full specification of state variables such as temperature, pressure, initial composition, system size, etc. An equilibrium calculation is normally done in POLY-3 according to the *Global Minimization Technique*, which ensures that the most stable minimum under the specified conditions is computed.

For an equilibrium calculation to be performed, the state variables must all be set as conditions for the calculations. Such conditions include, for example, temperature, pressure, and system composition. When you calculate an equilibrium in the POLY module, you have to set these conditions manually.

Setting Conditions

Setting a condition normally involves giving a single state variable a specific value. For example, you can set the temperature to 1273.5 Kelvin (T=1273.5). Alternatively, setting a condition can involve giving a linear expression with more than one state variable a specific value. For example, you can set the mole fraction of the S component to be the same in the liquid and the pyrrohotite phases (`X(LIQ,S)-X (PYRR,S)=0`).

The number of state variables that need to set is determined by the *Gibbs Phase Rule*. Typically, the state variables to give values to are:

- temperature (in K)
- pressure (in Pascal)
- system size in number of moles (in mole) or mass (in grams)
- the fraction of each component (in number of moles or mass)

If you fix the phase of the equilibrium and all but one of the state variables, you can discover the value of the other state variable at equilibrium.

It is possible to specify a set of conditions that does not have any equilibrium and the program detects this by failing to reach equilibrium during the calculation.

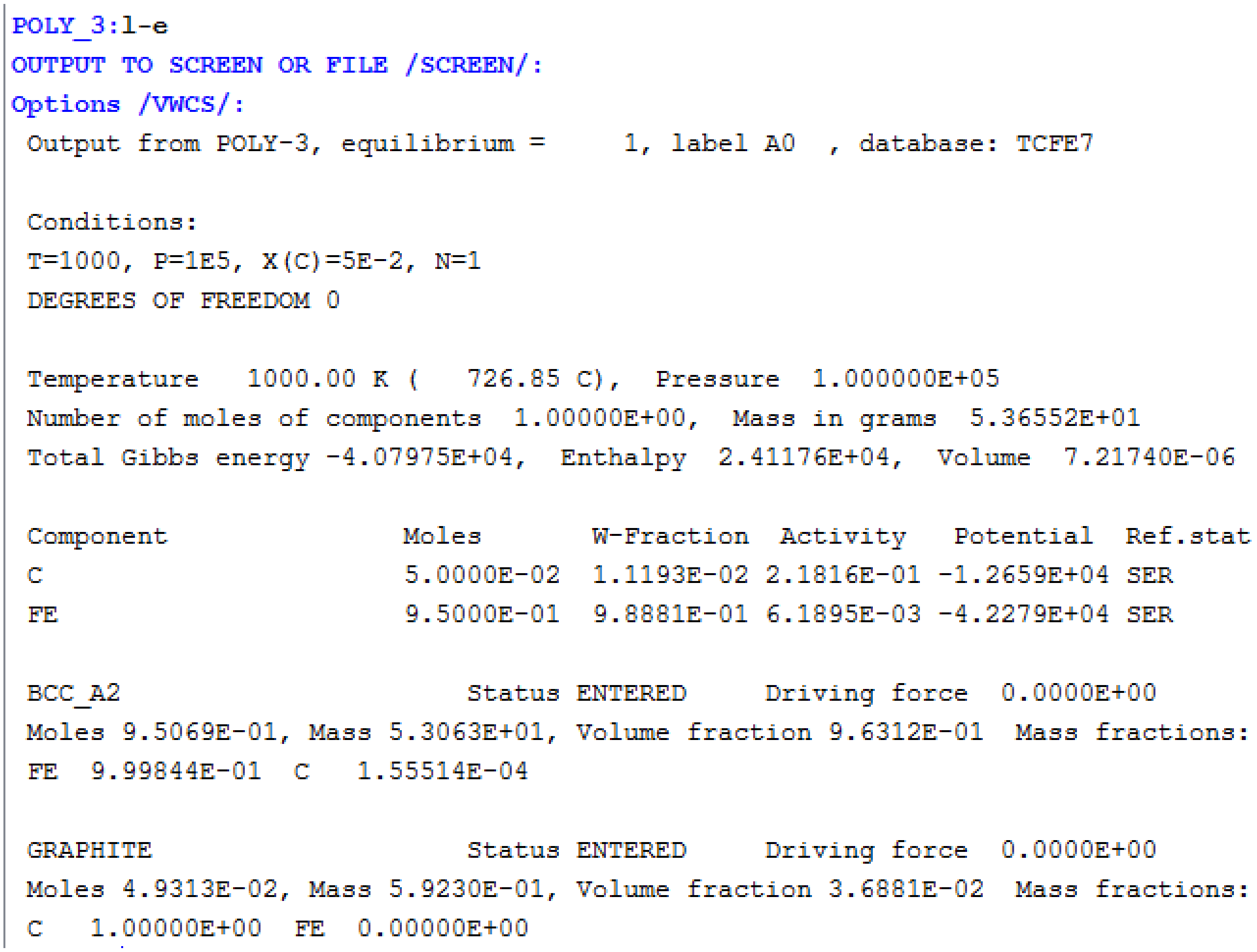
State Variables for Setting Conditions

The following table lists some of the available state variables you can use to set conditions:

State Variable	SET_CONDITION Parameter
temperature in the system (in K)	T
pressure in the system (in Pascal)	P
system size (mole number in moles)	N
system size (mass in grams)	B

State Variable	SET_CONDITION Parameter
number of moles of a component in the system	N(<component>)
mole fraction of a component in the system	X(<component>)
mass fraction of a component in the system	W(<component>)
activity of a component in the system	ACR(<component>)
chemical potential of a component in the system	MUR(<component>)
mole fraction of a component in a phase	X(<phase>,<component>)
mass fraction of a component in a phase	W(<phase>,<component>)
activity of a species referred to a phase at ambient temperature and pressure	ACR(<species>,<phase>)
chemical potential of a species referred to a phase at ambient temperature and pressure	MUR(<species>,<phase>)
enthalpy in the system (in J)	H
enthalpy of a phase (in J/mol)	HM(<phase>)

Equilibrium Information Example



```
POLY_3:l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1000, P=1E5, X(C)=5E-2, N=1
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.36552E+01
 Total Gibbs energy -4.07975E+04,  Enthalpy  2.41176E+04,  Volume  7.21740E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       5.0000E-02  1.1193E-02 2.1816E-01 -1.2659E+04 SER
 FE                      9.5000E-01  9.8881E-01 6.1895E-03 -4.2279E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.5069E-01, Mass 5.3063E+01, Volume fraction 9.6312E-01  Mass fractions:
 FE  9.99844E-01  C   1.55514E-04

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 4.9313E-02, Mass 5.9230E-01, Volume fraction 3.6881E-02  Mass fractions:
 C   1.00000E+00  FE  0.00000E+00
```

Calculating an Equilibrium

This topic explains how to calculate an equilibrium in POLY. To calculate an equilibrium means to calculate the equilibrium composition of your system, given a full specification of conditions that reduce the degrees of freedom of the calculation to zero.

If you are running a network client installation of Thermo-Calc and cannot enter the POLY module, this may be because all the license instances on that the license server makes available have been checked out.

Also see *POLY_3 Commands* on page 117 in the *Thermo-Calc Console Mode Command Reference*.

1. Define your system (see *Defining a System in Console Mode* on page 129).
2. Go to the POLY module. At the SYS prompt, type `GOTO_MODULE` and enter `POLY`.

3. Use SET_CONDITION followed by conditions and value assignments to set the conditions of your calculation. For example, to set temperature, pressure, initial composition and system size for a Fe-Cr-C system, you might enter the following:

   ```
   SET_CONDITION T=1200 P=1E5 W(CR)=0.18 W(C)=0.0013 N=1
   ```

   This sets the temperature (T) to 1200 K, the pressure to 1 bar (100,000 Pascal), the mass fraction of Cr to 18 mole percent, the mass fraction of C to 0.13 weight percent, and the total amount of material to 1 mole. The fraction of Fe in the system is calculated from the fractions of Cr and C. You have to set the fraction of all the components in your system except one.

4. Use COMPUTE_EQUILIBRIUM to run the calculation.
5. Use LIST_EQUILIBRIUM to see the results of the calculation.

Calculating an Equilibrium with a Fixed Phase

There are many ways to calculate equilibriums in Thermo-Calc. The following is one example.

You can calculate an equilibrium that has a certain amount of a certain stable phase. Use *CHANGE_STATUS* on page 59 and choose `Phase` to specify the phase and the amount of that phase (in normalized mole number) that you want to set as fixed. For example, if you want to find out at what temperature a system starts to melt, enter the following:

```
CHANGE_STATUS PHASE LIQUID=FIX 0
```

You must leave the state variable whose equilibrium value you are interested in unspecified. However, if you have already specified that state variable, you can make it unspecified again by using *SET_CONDITION* on page 165 and set that state variable to `NONE`. For example, if you have given temperature a value, you can type:

```
SET_CONDITION T=NONE
```

The calculated equilibrium includes the value of the unspecified variable at which the equilibrium enters the phase that is fixed.

For an example where an equilibrium is calculated with a fixed phase, see Example 7 in *Console Mode Example Collection* on page 14.

Calculating an Equilibrium with Suspended or Dormant Phases

You can calculate an equilibrium under the assumption that one or several phases are `SUSPENDED` or `DORMANT` using CHANGE_STATUS and choose `Phase`. For example, to specify that all phases except one should be suspended, you can first suspend all phases and then enter a single phase in the following way:

```
CHANGE_STATUS PHASE *=SUSPENDED
CHANGE_STATUS PHASE FE_LIQUID=ENTERED
```

For an example where this is done, as well as where the status of phases is set to be dormant, see Example 10 in *Console Mode Example Collection* on page 14.

Property Diagrams

In this section:

About Property Diagrams

When you calculate and plot a property diagram, there is only one independent state variable. Many different properties can be plotted as a function of this independent variable. For example, if the independent state variable is temperature, then the mole fractions of all phases can be plotted as a function of temperature. Or the composition of a specific phase may be plotted relative to temperature, or the activity of a component in the system as a whole or in a specific phase may be plotted relative to it.

A property diagram is plotted based on a series of equilibria that is computed while the value of one state variable is varied between a minimum and a maximum value. This variable is referred to as the stepping axis variable. In Thermo-Calc, first calculate one initial equilibrium, and then new equilibria are calculated at incremental steps in both directions on the stepping axis from the initial equilibrium. This continues until the stepping operation has covered the length of the axis between a minimum and a maximum value that is specified.

For an example of the calculation of a property diagram, see Example 8 in *Console Mode Example Collection* on page 14.

Calculating and Plotting a Property Diagram

This topic explains how to calculate a property diagram in POLY. To calculate a property diagram means to calculate a series of equilibria while the value of the stepping axis variable varies between a minimum and a maximum value. With the exception of the stepping axis variable, all the state variables that you set when you calculate the initial equilibrium retain the values when the new equilibria are calculated.

POLY_3 Commands on page 117 in the *Console Mode Command Reference*.

How to Calculate and Plot a Property Diagram

1. Calculate an initial equilibrium in the POLY module (see *Equilibrium Calculations* on page 132).
2. Use SET_AXIS_VARIABLE to set the axis variable, the minimum and the maximum stepping variable values and the step length. The first parameter of SET_AXIS_VARIABLE is the axis number. Since a property diagram only has one axis variable, this is set to 1. For example, if you want to set the axis variable to temperature, and calculate an equilibrium at every 50 K between a minimum temperature of 100 K and a maximum temperature of 2000 K, enter

   ```
   SET_AXIS_VARIABLE 1 T 100 2000 50
   ```

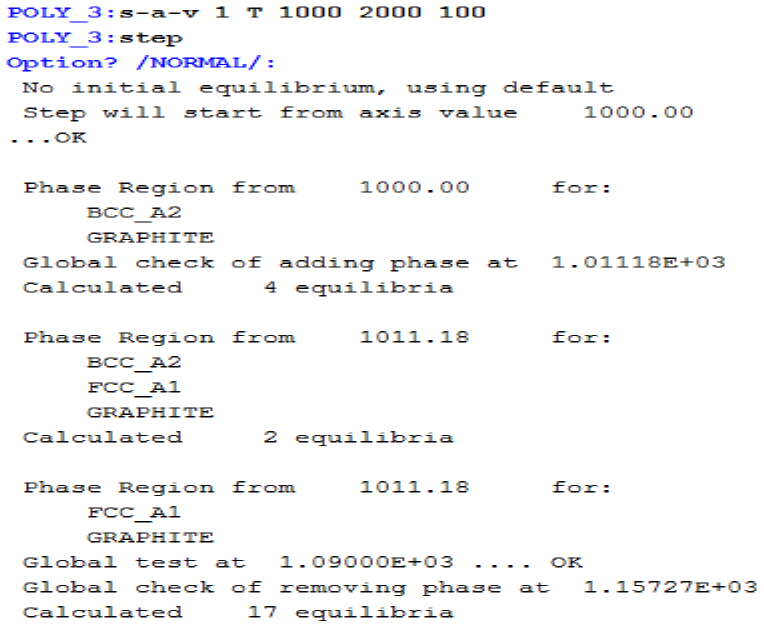
An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable. Also, the minimum stepping variable value must be smaller than, and the maximum value larger than, the value that you set the state variable to when calculating the initial equilibrium.

3. Use STEP_WITH_OPTIONS and choose `Normal` to perform the stepping operation.

Thermo-Calc lists the phase regions along the stepping axis, the phases contained in each region, and the number of equilibria calculated in that region. Each region is defined by the phases it contains.

The number of equilibria calculated is not just the number of steps that are performed according to the step length and the minimum and maximum values on the axis variable. This is because Thermo-Calc calculates extra equilibria when a new phase is discovered in order to determine the phase region boundary more precisely.

Step with Options Example



```
POLY_3:s-a-v 1 T 1000 2000 100
POLY_3:step
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    1000.00
...OK

 Phase Region from    1000.00      for:
     BCC_A2
     GRAPHITE
 Global check of adding phase at  1.01118E+03
 Calculated      4 equilibria

 Phase Region from    1011.18      for:
     BCC_A2
     FCC_A1
     GRAPHITE
 Calculated      2 equilibria

 Phase Region from    1011.18      for:
     FCC_A1
     GRAPHITE
 Global test at  1.09000E+03 .... OK
 Global check of removing phase at  1.15727E+03
 Calculated     17 equilibria
```

4. To plot the diagram, use POST to open the POST module and then use PLOT_DIAGRAM. By default, the X-axis represents the stepping axis variable and Y-axis represents the sum of the mole fractions of all phases (NP(*)).

Calculating a Property Diagram One Phase at a Time

There are many ways to calculate property diagrams in Thermo-Calc. One example is where you can calculate a property diagram with a separate stepping operation being performed for each phase at a time in its default most stable composition (the major constitution). This is useful if you want to create a property diagram for a heterogeneous system with both ordered phases and their disordered pairs.

To calculate a property diagram one phase at a time, use *STEP_WITH_OPTIONS* on page 172 and when prompted choose `One_phase_at_time` to perform the stepping operation.

Calculating Several Properties in the Same Diagram

There are many ways to calculate property diagrams in Thermo-Calc. The following is another example. If you perform several stepping calculations after each other, the results of these calculations are all saved in your workspace file. This allows you to the following:

- Calculate (and then plot) missing parts of a specific property inside the first property diagram. These parts are calculated inside the range of the stepping variable with a different control condition.
- Calculate (and then plot) two or more sets of a specific property on the same property diagram for the same system. These can be calculated under different control conditions with stepping operations being performed across the same stepping axis variable range.
- Calculate phase boundary lines and then plot them in a corresponding phase diagram for the same system. This can be especially useful for some defined secondary phase-transformations. For example, if you want to find the phase boundary between BCC_A1 and BCC_B2, or the equal-Gm for two specific phases, or the equal-fraction or equal-activity for two specific phases of a certain species, then this can be useful.

Unless you have opened a new workspace file previously using SAVE_WORKSPACES , the results of the stepping calculations are saved in a RESULT.POLY3 file. To save the results of several stepping calculations in a file different from the workspace file that your results are currently saved to, then use SAVE_WORKSPACES before you perform the first stepping calculation.

SAVE_WORKSPACES overwrites and deletes the results of all previous stepping calculations.

Phase Diagrams

In this section:

About Phase Diagrams

Phase diagrams have two or more independent axis variables. Any state variable that has already been set can be used as the mapping variable for a mapping calculation and then as the axis variable for a phase diagram. From a mapping calculation, many types of phase diagrams can be plotted, with one of the mapped variables as one axis variable, and with other mapped variables or any varied property (state or derived variables) or entered symbol (variables, functions or table values) as the other axis variables.

All phase diagrams consist of zero phase fraction lines. There are two distinct types of phase diagrams: those with the tie-lines in the plane of the diagram and those where the tie-lines are not in the plane. The former includes binary phase diagrams and ternary isotherms. The latter includes more general isopleth diagrams with one or more fixed extensive variables (normally, this is a composition). The BIN and TERN modules calculate binary and ternary phase diagrams. The POTENTIAL and POURABIX modules calculate the more general isopleth diagrams and other related diagrams.

The following topics describe how to calculate the types of phase diagrams in the *POLY_3 Commands* on page 117 module. In POLY, you can calculate phase diagram for systems with up to 40 components and with thousands of phases. You can combine activity conditions and fixed phase status and fraction conditions in any way. Thermo-Calc can calculate any arbitrary 2D section through composition space.

There is no guarantee that the conditions set will result in a calculation that reaches an equilibrium.

For an example of the calculation and plotting of a phase diagram, see Example 4 in *Console Mode Example Collection* on page 14.

Calculating and Plotting a Phase Diagram

This topic describes how to calculate a phase diagram in the POLY module. The commands are described in *POLY_3 Commands* on page 117 and *POST Commands* on page 188.

1. Calculate an initial equilibrium in the POLY module (see *Equilibrium Calculations* on page 132).
2. Use SET_AXIS_VARIABLE to set the first axis variable, its minimum and maximum mapping value and the length of each incremental step on this axis. The first parameter of SET_AXIS_VARIABLE is the axis number and is set to 1. For example, suppose you want the mass fraction of C as your first axis variable. You want it to vary between 0 and 0.1, with the length of each incremental step being no more than 0.002. You then enter:

   ```
   SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
   ```

An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable.

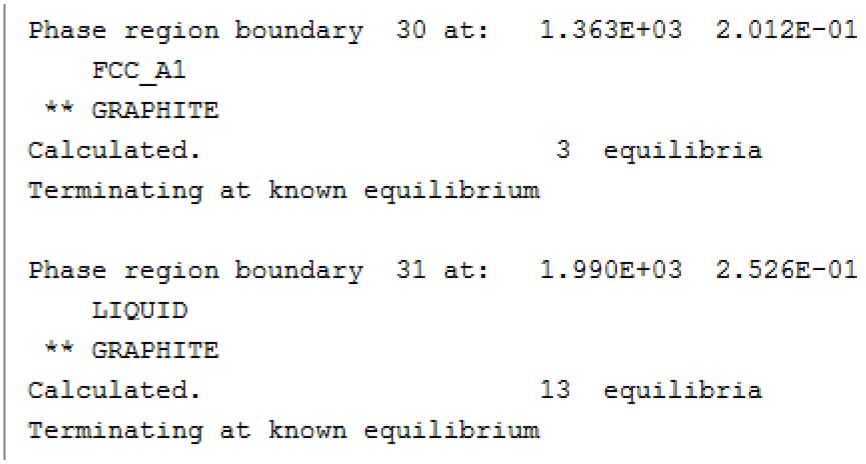
3. Use SET_AXIS_VARIABLE to set the second axis variable and specify its minimum, maximum, and step length values. The axis number is set to 2. For example, suppose you want temperature as your second axis variable and you want it to vary between 900 K and 1900 K, with an incremental step of 25 K. You then enter:

   ```
   SET_AXIS_VARIABLE 2 T 900 1900 25
   ```

4. If you want more than two axis variables, then use SET_AXIS_VARIABLE until you have set all the axis variables. You can set up to five axis variables. Axis variables 3, 4 and 5 must be set temperature, pressure or to the chemical potentials of components.

   You may want to save your workspace with SAVE_WORKSPACES before you perform the mapping calculation. This saves the axis variables you have set. However, it overwrites the results of any previous stepping or mapping calculations done.

5. Use MAP to perform the mapping calculation. The console lists the phase region boundaries and the phases contained on one side of each boundary.



```
Phase region boundary  30 at:   1.363E+03  2.012E-01
    FCC_A1
 ** GRAPHITE
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   1.990E+03  2.526E-01
    LIQUID
 ** GRAPHITE
Calculated.                     13  equilibria
Terminating at known equilibrium
```

6. To plot the diagram, use POST to open the POST module and then use PLOT_DIAGRAM. By default, the X-axis represents mapping axis variable 1 and the Y-axis represents mapping axis variable 2.

Calculating a Quasi-Binary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example where a quasi-binary phase diagram is used for calculations on a ternary system in which one component has an activity or chemical potential that is fixed (although if you have fixed a phase and the phase composition varies, then the activity or chemical potential may also vary). The tie-lines in a quasi-binary diagram are in the diagram's plane of the diagram. This means that the calculation follows the lever rule as well as other rules.

For an example of a calculation of a quasi-binary phase diagram, see Example 17 in *Console Mode Example Collection* on page 14.

How to Calculate a Quasi-Binary Phase Diagram

Use CHANGE_STATUS to set the component that has a fixed activity or chemical potential. For example, suppose you want to compute a phase diagram for a Ca-Fe-O system in which the liquid oxide (`FE-LIQ`) is in equilibrium with liquid Fe. You then enter:

```
CHANGE-STATUS FE-LIQ=FIX 0
```

Calculating a Quasi-Ternary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example of a quasi-ternary phase diagram used for calculations on a quaternary system where one component has a fixed activity or fixed chemical potential.

How to Calculate a Quasi-Ternary Phase Diagram

When calculating a quasi-ternary phase diagram it is necessary to set a condition on either activity or chemical potential of the fourth component. To specify a meaningful value it is recommended that you first change the component's reference state using SET_REFERENCE_STATE. For example, to calculate a phase diagram for a quasi-ternary Fe-Cr-Ni-C system with fixed carbon activity, you can enter the following:

```
SET_REFERENCE_STATE C GRAPH ,,
```

You must also use SET_CONDITION to set the activity of the component whose activity or chemical potential you have fixed. Do this by assigning a value to the ACR state variable. For example, if the component is carbon, you might enter

```
SET_CONDITION ACR(C)=0.002
```

Scheil Simulations

In this section:

About Scheil Simulations

Thermo-Calc is primarily a program for performing equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can be simulated. One example of such a transformation is a Scheil-Gulliver solidification.

In a Scheil-Gulliver solidification, the diffusion in the solid phases is assumed to be so slow that it can be ignored, while the diffusion in the liquid phase is assumed to be very fast. With this approximation, the conditions at the liquid/solid interface can be described as a local equilibrium.

By making a stepping operation on the temperature variable (or enthalpy or amount liquid phase) with small decrementing steps, the new composition of the liquid can be determined. After each step, the amount of formed solid phase is removed and the overall composition is reset to the new liquid composition. In effect, the whole system is described as a non-equilibrium state regarding various parts of solidified phases at various solidification stages.

The Scheil Module

You can simulate Scheil-Guilliver solidification processes with the SCHEIL module. When you enter the module, you are prompted to answer a series of questions about which database to use, what the major element is and in which amount. Thermo-Calc then displays a property diagram showing how the fraction of solid phase varies with temperature (in Celsius). You can then plot diagrams using other variables you are interested in. Do this by starting a new simulation, by opening an old file with the results of a previous simulation that you can plot differently. For example, you might be interested in plotting the fraction of remaining liquid against temperature, the fraction of each solid phase or the total of solid phases against temperature, the microsegregation in each solid phase, or the latent heat evolution against temperature.

It is possible to use the SCHEIL module to run a modified Scheil-Gulliver simulation that also takes back-diffusion of some fast-diffusing interstitial elements such as C or N into account, as well as BCC to FCC phase transformation phenomena.

Scheil Module Examples

- See Examples 15 and 30 to simulate non-equilibrium transformations without considering fast-diffusion elements.
- See Example 48 to simulate partial-equilibrium transformation with fast-diffusion elements taken into consideration. This example also shows how you can perform lever-rule calculations (full-equilibrium transformations).

Scheil and the Diffusion Module (DICTRA)

If you also have a license for the Diffusion Module (DICTRA), you can import a previously calculated Scheil segregation profile into the software using the command INPUT_SCHEIL_PROFILE. Search the online help or see the *Diffusion Module (DICTRA) Command*

Reference.

Simulating a Scheil-Solidification

Simulating a Scheil-Gulliver solidification process involves calculating the liquid composition of a higher-order multicomponent system at each step of a cooling process, and resetting the liquid composition as the composition of the entire system (after having removed all amount of solid phase).

SCHEIL Commands on page 235 in the *Console Mode Command Reference*.

How to Simulate a Scheil-Solidification

1. Use GOTO_MODULE SCHEIL to enter the SCHEIL module.
2. Type START-WIZARD.
3. Specify which `Database` to use.
4. Specify the `Major element or alloy` in your system.

   For example, for a steel/Fe-alloy, enter `Fe`, for an Al-based alloy, enter `Al`, and for a Ni-based super alloy, enter `Ni`.

5. Set whether to specify the `Composition input in mass (weight) percent` (the default) or in `Mole percent`. Enter `Y` for mass percent and `N` for mole percent.
6. Specify the name of the `1st alloying element`. You can directly specify mass or mole percent after the name (for example, enter `Cr 5`). If this is not specified, then you are prompted to enter it separately.
7. Specify the other alloying elements in the same way as you specify the first (for example, `c 1`).
8. After you have specified your last alloying element, press <Enter> when requested to specify the next element. This ends the process of defining the bulk composition of the alloy system.

   You can also specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element in Step 6. For example, you can enter `Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02`.

9. Specify the starting `Temperature (C)` in Celsius. The default is `2000`.

   This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.

10. Decide which phases (if any) to reject at the `Reject phase(s)` prompt. Enter the name of the phases to reject or press <Enter> for `NONE`.
11. Decide whether to `Restore phase(s)`. You may want to restore a phase that you rejected when you ran the simulation earlier, or you may want to restore a phase that is rejected by default in your database. Enter the name of the phases to restore or press <Enter> for `NONE`.
12. When prompted `OK?` type `N` to go back to Step 9 to reconsider which phases to reject or restore. Type `Y` to continue.

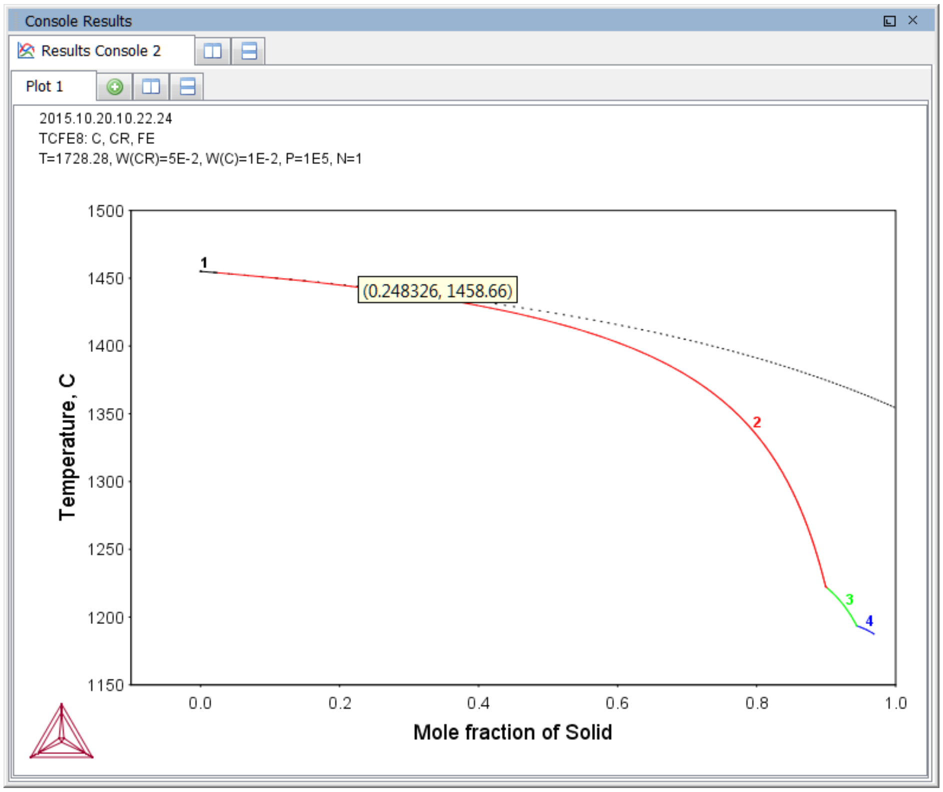
    Thermodynamic data about the alloy system you defined is retrieved from the database.

13. At the `Should any phase have a miscibility gap check` prompt, press <Enter> for `N` or answer `Y`.

    If you answer `Y`, you are prompted to specify the `Phase with miscibility gap`. Answer with a solution phase name(s) (in this example `FCC` is entered) as well as the `Major constituents for sublattice` (for each sublattice site) (for this example, `Cr` is entered for sublattice 1 and `C` for sublattice 2). In this example the `Phase with miscibility gap` is `LIQUID PHASE NAME: LIQUID`.

14. Press <Enter> to specify another phase.
15. Specify the names of any `Fast-diffusing components`. Press <Enter> for `NONE` or type all the names on the same line then press <Enter>. If you do specify any fast-diffusing components, then you are prompted to set whether BCC to FCC phase transformations should be simulated.

    The Scheil-Gulliver solidification simulation runs, and the default diagram (Temperature versus Mole Fraction of Solid) is automatically plotted in the Console Results window.



```
2015.10.20.10.22.24
TCFE8: C, CR, FE
T=1728.28, W(CR)=5E-2, W(C)=1E-2, P=1E5, N=1
```

Plotting Additional Scheil Simulation Diagrams

Post processing is done the same way as POLY-3 (see *POLY_3 Commands* on page 117), specific variables for plotting in the Scheil Module are listed.

Abbreviations for Scheil State Variables

The variables can be plotted along the X- and Y-axes. In the table, *ph* is an abbreviation of *phase*, and *el* is an abbreviation of *element*. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram.

Abbreviation	**State variable**
T	Temperature in Celsius
NL/BL	Mole/mass fraction of liquid
NS/BS	Mole/mass fraction of all solid phases
NS(ph)/BS(ph)	Mole/mass fraction of a solid phase
W(ph,el)	Weight fraction of an element in a phase
X(ph,el)	Mole fraction of an element in a phase

Abbreviation	State variable
Y(ph,el)	Site fraction of an element in a phase
NN(ph,el)	Distribution of an element in a phases
NH/BH	Heat release and Latent heat per mole/gram
CP/BCP	Apparent heat capacity per mole/gram
NV/NV(ph)	Molar volume of the system or a phase
DS/DS(ph)	Average density of the system or a phase
BT	Apparent volumetric TEC of the system

T0 Temperature Simulations

In this section:

T0 Temperature Simulations

The T0-temperature is the temperature at which two phases have the same Gibbs energy for a certain composition in a multicomponent system. The T_0-temperature is located within the two-phase field between the phases and it is the theoretical limit for a transformation without diffusion. T0-temperatures are often of interest if you want to understand how diffusionless transformations work. The T0 temperature in a multicomponent system with a fixed composition is temperature at which the tangent lines of the Gibbs energies of the two target phases are the same.

If the composition of one or two components varies, the common Gibbs energy for the two phases in partial equilibrium of a diffusionless transformation becomes a plane or surface, and the T0 temperature becomes a line or plane.

See Examples 23 and 41 in the *Console Mode Examples*.

Also see *Making a T0 Temperature Simulation* below for step-by-step instructions. as well as *Console Mode POST Module* on page 181.

Making a T0 Temperature Simulation

This describes how to perform a T0 temperature simulation and apply a stepping calculation to its initial result.

Before you perform a T0 temperature calculation, you must have defined your initial system and be in POLY. The initial overall composition must have appropriate settings for the desired T0 temperature calculation for the two target phases.

See *POLY_3 Commands* on page 117 in the *Thermo-Calc Console Mode Command Reference*.

How to Make a T0 Temperature Simulation

1. Use SET_CONDITION to set the conditions of your calculation in the same way as when you calculate an ordinary equilibrium.
2. Use COMPUTE_EQUILIBRIUM to run the calculation. The calculation does not need to reach an equilibrium in which any of the target phases is stable.
3. When you have calculated your initial equilibrium, use ADVANCED_OPTIONS and choose `T-zero`.
4. When prompted, specify the names of the two target phases for which the T0 temperature (where the phases’ Gibbs energies are equal) is to be calculated.
5. If the T0 temperature between the two target phases is calculated, this temperature (in

Kelvin) is shown in the Console window.

6. If you want to do a stepping calculation based on this initial T0 temperature calculation, then use SET_AXIS_VARIABLE to specify which state variable to use as the stepping variable. This is done the same way as when you calculate a normal property diagram.

When a T0 temperature simulation is run, you cannot set temperature as the stepping variable.

7. Use STEP_WITH_OPTIONS and choose `T-zero` to initiate the stepping calculation. You are prompted to specify the names of the target phases for which the T0 temperature is calculated.

During the STEP T-ZERO calculation procedure, the calculated T0 values are presented next to the stepping variable.

For example, part of the output might look like this:

```
Phase Region from   1.000000E-01 for:
BCC_A2
FCC_A1
1.000000E-01         940.24
9.250000E-02         941.20
2.500000E-03         977.61
7.500000E-09         979.34
```

When the stepping calculation has finished, you can move to the POST module and plot the T0 line against the stepping composition variable or another varying axis value. Or you can impose the calculated T0 line onto a normal phase diagram.

Paraequilibrium

In this section:

About Paraequilibrium

A paraequilibrium is a partial equilibrium where one interstitial component (such as carbon C and nitrogen N) in a multicomponent alloy can diffuse much faster than the other components (the substitutional elements, including the matrix element and alloying elements). The chemical potential for the interstitial component in two partially equilibrated phases is equal in such a case, but this is not true for the other components. In such a paraequilibrium state, it is possible to have a transformation that is partly without partitions, where a new phase of the mobile component can form with different content but where the slowly diffusing components retain their compositions.

A paraequilibrium calculation is useful when, for example, you want to study phase transformations in systems with large differences in the diffusivities of different elements. Transformations occurring under paraequilibrium states can be much more rapid than if full local equilibrium holds at the phase interface.

See Example 42 in the *Console Mode Examples*.

Also see *Calculating a Paraequilibrium* below for step-by-step instructions.

Calculating a Paraequilibrium

This topic describes both how to calculate an initial paraequilibrium with two target phases, and how to base a stepping calculation on this initial calculation.

Before you do any paraequilibrium calculations, you must have defined your initial alloy system and be in POLY. The initial overall composition must have appropriate settings for the desired paraequilibrium calculation for the two target phases.

How to Calculate a Paraequilibrium

These commands are described in the *Thermo-Calc Console Mode Command Reference* included with this documentation set.

1. Use SET_CONDITION to set the conditions of your calculation just like when you calculate an ordinary equilibrium.
2. Use CHANGE_STATUS to set the status of the chosen interstitial components to SPECIAL. For example, if C is an interstitial component, enter:

   ```
   CHANGE_STATUS COMPONENTS C=SPECIAL
   ```

   This gives you a clear picture on u-fractions of the substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that the specified components are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

3. Use COMPUTE_EQUILIBRIUM to run the calculation.
4. When you have calculated your initial equilibrium, use ADVANCED_OPTIONS `Paraequilibrium` to perform the paraequilibrium calculation.
5. Specify the names of the target phases of the paraequilibrium state. For example, `FCC#1 BCC` and `FCC#2 M23C6`.

Both phases must have similar interstitial/vacancy sublattices that the fast-diffusion interstitial components occupy. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system.

6. Specify the names of one or more fast-diffusing components. These components must be located on the interstitial/vacancy sublattices in both of the chosen phases.

Interstitial components (for instance C and N combined) may have significantly different behaviours depending on how they are partitioned in different structured phases.

If the paraequilibrium between the two specified phases is successfully calculated, then a message is displayed, for example:

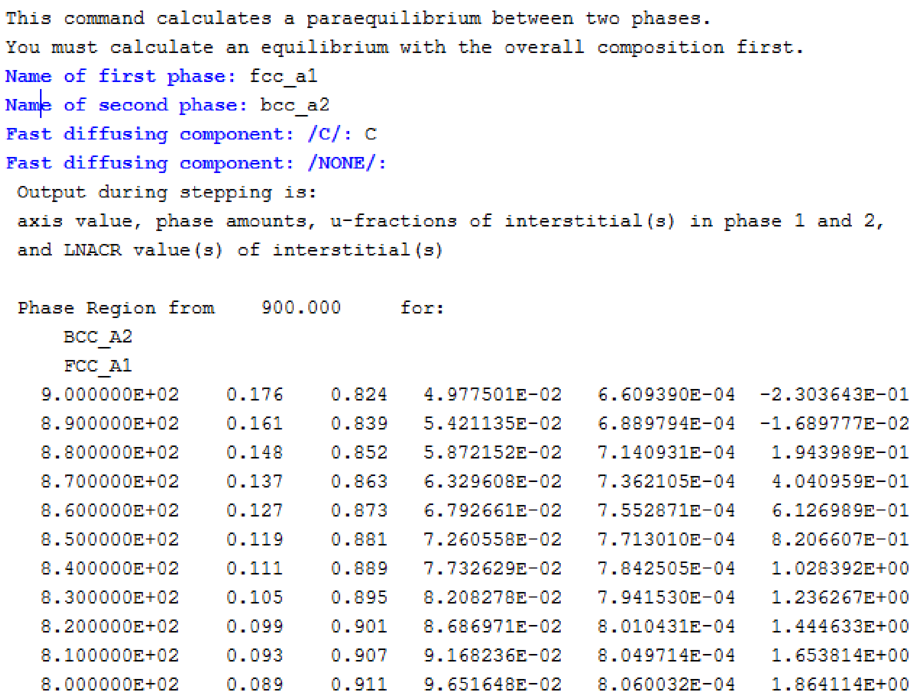
```
NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02 N = 4.1548129E-03
NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04 N = 2.3781027E-04
All other compositions are the same in both phases
```

The first two lines show the phase amounts expressed in mole-percent [NP(phase)] and the contents of the interstitial components C and N in each phase. These contents are expressed in u-fractions. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) are equal in the two target phases at the paraequilibrium state.

7. If you want to do a stepping calculation based on this initial paraequilibrium, then use SET_AXIS_VARIABLE to specify which state variable to use as the stepping variable. This is done exactly in the same way as when you calculate a normal property diagram.
8. Use STEP_WITH_OPTIONS → `Paraequilibrium` to initiate the stepping calculation. You are prompted to specify the names of the target phases of the paraequilibrium states as well as the fast-diffusing components.

The stepping calculation is performed, and the different phase regions are listed with columns for the value of the stepping variable, the amounts of the two target phases, the u-fractions of interstitial(s) in each of the two phases, and the LNACR value(s) of the interstitial component(s).

Example



```
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824   4.977501E-02   6.609390E-04  -2.303643E-01
   8.900000E+02    0.161    0.839   5.421135E-02   6.889794E-04  -1.689777E-02
   8.800000E+02    0.148    0.852   5.872152E-02   7.140931E-04   1.943989E-01
   8.700000E+02    0.137    0.863   6.329608E-02   7.362105E-04   4.040959E-01
   8.600000E+02    0.127    0.873   6.792661E-02   7.552871E-04   6.126989E-01
   8.500000E+02    0.119    0.881   7.260558E-02   7.713010E-04   8.206607E-01
   8.400000E+02    0.111    0.889   7.732629E-02   7.842505E-04   1.028392E+00
   8.300000E+02    0.105    0.895   8.208278E-02   7.941530E-04   1.236267E+00
   8.200000E+02    0.099    0.901   8.686971E-02   8.010431E-04   1.444633E+00
   8.100000E+02    0.093    0.907   9.168236E-02   8.049714E-04   1.653814E+00
   8.000000E+02    0.089    0.911   9.651648E-02   8.060032E-04   1.864114E+00
```

It is possible to now move to the POST module and plot some of the results of the calculation. For an example of a paraequilibrium calculation and how it can be plotted, see Example 23 in the *Console Mode Examples*.

Potential Diagrams

In this section:

About Potential Diagrams

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

This topic describes how to calculate such potential diagrams with the POTENTIAL module, and how to later modify the pressure of such a calculation in POLY. The calculation done by the POTENTIAL module always assumes a pressure of 1 bar.

POTENTIAL_DIAGRAM Module on page 217 in the *Console Mode Command Reference*.

Calculating a Potential Diagram

You need access to a substance or solution database that contains a gaseous mixture phase, metals (or alloys), and solids such as metal-oxides, sulphides, sulphates, carbonates, silicates, nitrides or nitrates (stoichiometric or solution phases).

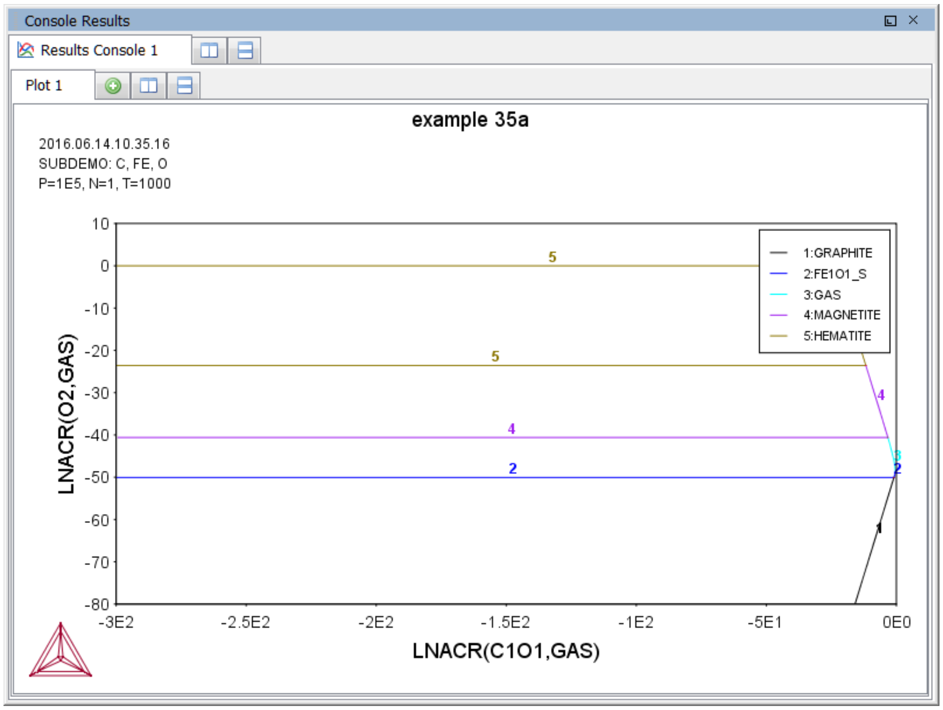
POTENTIAL_DIAGRAM Module on page 217 in the *Console Mode Command Reference*.

1. Use GOTO_MODULE and enter `POTENTIAL`.
2. Specify which substance or solution database to use. Any substance or solution database can be used that has a gaseous mixture phase, metals (or alloys), and solids such as metalxides, sulphides, sulphates, carbonates, silicates, nitrides, and nitrates (stoichiometric or solution phases).
3. Specify the matrix element (a metal) and the two gaseous species that define you metal-gas interaction system. The names of these components must be available in the database you are using.
4. Set the temperature (in Kelvin). (The pressure is always 1 bar.)

A potential diagram with the activities of the two gaseous species as mapping variables is calculated. These mapping variables are also set as the axis variables in the plotted diagram.

Example Plot

The following is an example diagram (from example 35 in the *Console Mode Examples*).



A POLY3-file is also automatically saved in the current working directory with the default name POT.POLY3.

5. When the diagram is plotted, it opens the POST module where you can modify the plotted diagram in any way you like.

Calculating a Potential Diagram with Different Pressure

It is possible to modify both the calculation and the plotted diagram that the POTENTIAL module generates in the POLY and POST modules. You can do this by opening a POLY3-file with the results from a POTENTIAL module calculation in either POLY or POST. You can modify the calculation in the same way that you can modify any ordinary mapping calculation or phase diagram. For example, this is useful for calculating a potential diagram at a pressure other than 1 bar.

POLY_3 Commands on page 117 in the *Console Mode Command Reference*.

You must have calculated a potential diagram already, and have the saved POLY3-file available.

1. Use GOTO_MODULE and enter `POLY`.
2. Use READ followed by the name of the POLY3-file that contains the results of the potential diagram calculation that you want to modify.

3. This opens the workspace file and loads the previous settings and results. The activities of the two gaseous species is now part of the conditions, and these conditions are set as the mapping variables.
4. Use SET_CONDITION to specify the pressure under which you want the potential diagram to be calculated. For example, to set the pressure to 1000 bar, enter:

   ```
   SET_CONDITION P=1e8
   ```

5. Use COMPUTE_EQUILIBRIUM to compute the initial equilibrium.

   You may also want to use ADD_INITIAL_EQUILIBRIUM to calculate some additional equilibria that the mapping calculations are based on.

6. Use MAP to perform the mapping calculations.
7. Use GOTO_MODULE and enter `POST` to set conditions for visualization and to plot the diagram.

Aqueous Solutions

In this section:

About Aqueous Solutions

Heterogeneous equilibrium calculations involving aqueous solutions are not different from other equilibrium calculations, but the setup of the equilibrium conditions and the reference states of the system is more complex. For example, the pH and Eh values of the aqueous solution phase are normally complex functions of bulk composition, temperature and pressure conditions.

For some simple systems, thermodynamic approximations of pH-Eh calculations can be used. But Thermo-Calc also has comprehensive thermodynamic models and databases for various non-ideal solution phases. These let you accurately calculate pH and Eh property diagrams (and many other types of property diagrams) in complex aqueous solutions in a variety of conditions.

A Pourbaix diagram is a pH-Eh phase diagram where the tie-lines are not in the plane. The chemical potentials or activities of two system components (H+ and EA) are used as mapping variables and the pH and Eh quantities are normally plotted on the X- and Y-axes of the diagram. You can use many other properties as axis variables in various property diagrams for the interaction system at a specific temperature and pressure. The phase relations between the aqueous solution and various metal forms, oxides, hydroxides, sulphides, sulphates, nitrates, silicates, carbonates and other solids, or gaseous mixtures, are represented as different fields defined by acidity and electric potential.

You can calculate Pourbaix diagrams with the Pourbaix module. The compositional definition and variations and the basic solvent and electron components H2O, H+1 and ZE are automatically determined by the aqueous solution phase in the Pourbaix module.

Key Components

These key components are defined as follows:

Component	Component status	Reference state	Ref-T(K)	Ref-P(Pa)
H2O	ENTERED	AQUEOUS	*	100000
H+1	ENTERED	SER		
ZE	ENTERED	REFERENCE_ELECTRODE	*	100000

Besides the aqueous solution phase, your system may also contain a gaseous mixture phase. Other neutral and charged gaseous species may also be constituents. For multicomponent systems there are normally also some interacting solid phases (stoichiometric or solution) as the so-called secondary phases. These are typically the matrix and/or precipitate phases in the alloys of interest.

Some databases have been specially developed for the Pourbaix module's diagram calculations. Such a database contains all necessary phases, i.e., an aqueous solution phase, a gaseous mixture phase, some alloy solid solution phases and some secondary solid phases. Databases developed for the Pourbaix module include *PAQ* (TCS Public Aqueous Solution Database) or *PAQS* (TGG Public Aqueous Solution Database).

If such a dedicated Pourbaix module is not used, then an aqueous solution database such as *TCAQ* (TC Aqueous Solution Database), *AQS* (TGG Aqueous Solution Database), or any user-specified aqueous databases can be used. This database contains at least the AQUEOUS and REFERENCE_ELECTRODE phases. The aqueous solution database needs to be appended with additional required data and phases, such as interacting alloy (solid) solution phases and secondary (solid and liquid) phases. Additional data is from one or more databases, such as SSUB/SSOL/TCFE or other substances/solutions databases.

Calculating a Pourbaix Diagram

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases.

When calculating a Pourbaix diagram, you need to have a database with an aqueous solution phase (that is, a phase with water as the dissolving solvent and with aqueous cation/anion and complex species as the dissolved solutes). Due to restrictions of aqueous solution models (SIT, HKF, Pitzer) used in the Thermo-Calc software, the aqueous solution database must be designed in the same Thermo-Calc database format as that used in the PAQ, PAQS, TCAQ and AQS databases for the aqueous solution phase.

Pourbaix diagram calculations are done in the advanced Pourbaix module.

POURBAIX_DIAGRAM Commands on page 219 in the *Console Mode Command Reference*.

How to Calcuate a Pourbaix Diagram

1. At the `SYS` prompt, enter GOTO_MODULE POURBAIX.
2. At the `Need any instruction on the POURBAIX module?` prompt, press <Enter> to skip or enter `Y` to learn more.
3. Press <Enter> at the prompt `Enforce a PAUSE after plotting when running a MACRO?`.
4. Press <Enter> to accept the default `1` to `Start a completely new POURBAIX diagram calculation` or enter `3` to `Open an old file and make another POURBAIX calculation`.

   To choose `3`, you must have already done a Pourbaix calculation and have it saved in a POLY3-file. The new calculation uses the same system definition as the previous calculation, but the other conditions, such as the bulk composition, temperature and pressure, can be modified in the next step.

5. Type `Y` or `N` to set whether to `Consider the GAS phase` (gaseous mixture phase) in the calculation.

The gaseous mixture phase should at least contain H2O, O2 and H2. If a GAS phase is not considered, then only the interactions between the aqueous solution phase and various solid phases (alloy phases and secondary phases) are calculated. Such a calculation may not accurately present all the heterogeneous interactions. Some secondary phases are therefore usually needed. Such phases exist in the PAQ or PAQS Public Aqueous Solution Databases. They can also be appended from the SSUB/SSOL/TCFE or other appropriate substances/solutions databases.

6. Type `Y` or `N` to set whether to `Use single database` (`Y`) or a multiple database (`N`).

   If you choose to use a single database, at the `Combined Database: /PAQ2/` prompt specify a database that is specially developed for the Pourbaix module’s diagram calculations.

   If you choose to use a multiple database, then you are prompted to specify an aqueous solution database and to append any additional required data and select necessary phases, such as various interacting alloy (solid) solution phases, and secondary (solid and liquid) phases, for example.

7. Specify all your solutes and the molality of each solute when prompted to do so. This can be done in terms of elements (such as Fe, Ni, Na, Cl, C or S) or arbitrary complex species (such as NaCl, CO2, CoCl3, Fe0.93S, NaSO4-1, or H2SO4). You can enter the element/species and the molarity on one line (for an example, NaCl 2.5).

> The first letter of the element abbreviation must always be upper case. Any second letters must be lower case. When you have finished your specification, press <Enter> when asked to specify `Next solute`.

The definition of your system and its initial bulk composition is now presented.

8. Type `Y` to confirm the defined system and its bulk composition.

   The thermodynamic data for your system is now retrieved from the database(s) chosen.

9. Answer the questions that you are prompted regarding various parameters of your calculation. You are asked to do any of the following:

- `Rejectphase(s)` or `Restore phases(s)`
- Check for miscibility gaps on any phase (`Should any phase have a miscibility gap check?`)
- `Enforce the Global Minimization Technique in calculations?`
- Save all functions, variables and tables in POLY3 file?
- `Set numerical limits` on the calculation

- Confirm defined conditions?
- Accept the default settings for two mapping variables

8. The Pourbaix calculation starts. Answer the question `Any missing phase boundary you could possibly think of?` Type `Y` or `N` to set whether you want to add starting points to the calculation. If you suspect that the calculation has missed some phase boundaries, this may help the program to detect them.
9. Answer questions about how the diagram is plotted and how to save the results of your calculation. You are asked to do any of the following:

- Change the pH/Eh steps for smoother curves?
- `Zoom in` on a specific region of the diagram
- `Change the curve-label option for the diagram`
- `Add label-texts onto the Pourbaix diagram`
- `Change the subtitle of the diagram`
- `Change the axis-texts`
- `Further refine the diagram in the POST Module`
- Print the diagram (save a `Hard copy of the diagram`)
- `Save the X-Y coordinates of curve on a text file`
- `Modify the diagram`
- Calculate and plot another Pourbaix diagram (`Any more diagram?`)

Plotting Additional Aqueous Solution Diagrams

When you have calculated a Pourbaix diagram, you can plot additional diagrams based on the results of the same calculation, but with different axis variables than Ph and Eh.

The variables can be plotted along the X- and Y-axes. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram. In the table, *AQsp* refers to the name of a specific aqueous species. The asterisk (*) can be used as a wild card character for all such species. If neither *AQsp* nor * is entered in parenthesis, then all species are searched.

You must have plotted a Pourbaix diagram to plot a diagram with other variables than Ph and Eh on the Y-axis and the X-axis. You can either plot such additional diagrams directly after having finished the plotting and saving/printing of a Poubaix Ph-Eh diagram or by choosing option `2` (Open an old file and plot other property diagrams) when you enter the POURBAIX module and opening a POLY3 workspace file.

Abbreviations for Aqueous Solution Variables

Abbreviation	Variable
pH	Acidity
Eh	Electronic Potential (V)
Ah	Electronic Affinity (kJ)
Pe	Electronic Activity (log10ACRe)
IS	Ionic Strength
TM	Total Concentration
Aw	Activity of Water
Oc	Osmotic Coefficient
MF(AQsp)	Mole Fractions of Aqueous Species
ML(AQsp)	Molalities of Aqueous Species
AI(AQsp)	Activities of Aqueous Species
RC(AQsp)	Activity Coefficients of Aqueous Species

How to Plot an Aqueous Solution Diagram

1. Type `Y` when prompted whether to plot any more diagrams, or select option 2 when you enter the POURBAIX module.
2. Specify which variable you want the X-axis to represent. Use the abbreviation specified in the preceding table. When you specify the name of an aqueous species, you can use the asterisk (*) to select all species.
3. Specify which variable you want the Y-axis to represent. The diagram is then automatically plotted.
4. Answer questions about how the diagram is plotted and how to save it. You are asked to do any of the following:

- change the axis-type (linear, logarithmic or inverse) on the X-axis or Y-axis
- zoom in on a specific region of the diagram
- change the curve-label option for the diagram
- add label-texts onto the Pourbaix diagram
- change the subtitle of the diagram
- change the axis-texts

- refine the diagram in the POST Module
- print the diagram (save a hard copy)
- save the X-Y coordinates of curve on a text file
- modify the plotted diagram
- calculate and plot another aqueous solution diagram

Stepping Calculations in an Aqueous Solution

Performing the stepping calculation overwrites all the previous settings and stepping results on the POLY3-file. To avoid this, use *SAVE_WORKSPACE* on page 232 to create a new workspace.

When you have calculated a Pourbaix diagram, you can use the saved results of the calculation (the POLY3-file), and make a property diagram based on stepping calculation.

Since the program normally sets the calculated initial equilibrium point as the starting point, the minimum value for the stepping variable must be specified as smaller or equal to the specific initial condition, and the maximum value as larger or equal to that condition. If pH is set as the stepping variable, the program automatically calculates the equilibrium constant in logarithmic (log10Ka) of the electrolysis reaction H2O (water) = H+ + OH- for the real aqueous solution under the current temperature-pressure-composition conditions, and thus this constant log10Ka value is considered as the highest pH in specifying the maximum value along stepping. Subsequently, confirm or modify an increment factor with a default value; for pressure and mole of a component, specify the step in logarithmic (log10P or log10N).

State Variable Abbreviations

You can use any of these state variables as a stepping variable.

State variable	**Abbreviation**
Temperature (K)	T
Pressure (bar)	P
Acidity	pH
Electronic potential (V)	Eh
Mole number of a dissolving component (such as Fe, Na, Cl, or NaCl) in 1 kg of water.	N(Comp) (for example, `N(Fe)`)

How to Do a Stepping Calculation

You must have plotted a Pourbaix diagram before making a stepping calculation on an aqueous solution.

1. Use GOTO_MODULE POURBAIX to enter the POURBAIX module.
2. Type `4` to Open an old file and make another STEPPING calculation.
3. Choose which POLY3-file to load.
4. Specify the conditions of the calculation by answering the questions that follows.

   The system definition is the same as in the previous Pourbaix calculation, but you can modify conditions such as bulk composition, temperature and pressure, and change some component definitions if necessary.

5. Specify which variable to use as the stepping variable (see the preceding table), its minimum and maximum value, and the length of each incremental step.

   The settings and stepping results are written to the opened POLY3-file, and a first default property diagram is plotted.

Pourbaix Examples TCEX40, 40A to 40E, and TCEX53

NOTES about TCEX40A and TCEX40E

In order to be able to subsequently run the TCEX40B (Main Option 2), TCEX40C (Main Option 3) and TCEX40D (Main Option 4), which open the previously-saved POURBAIX-type calculation POLY3 file, the user should make four copies of the resulting POURBAIX.POLY3 as TCEX40A.POLY3, TCEX40B.POLY3, TCEX40C.POLY3 and TCEX40D.POLY3.

However, this has to be properly done outsides of the TCCS software after the TCEX40A is executed. The reason is that, if saving the POLY3 workspace of the POURBAIX calculation results in the POLY3-module monitor (through the command sequence "GO PLOY3" and "SAVE TCEX40A.POLY3 Y"), all the initial equilibrium points and the mapping/stepping calculation results will be lost, and parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system) will be destroyed. In principle, before executing any Main Option (for calculations and graphical processing), it is highly recommended that the user shall save/rename/copy the previously-generated POLY3 file as another POLY3 file. Only in this way, it can avoid destroying the previous-saved POURBAIX-type calculation results.

Under Windows DOS-session (outside TCCS):

- copy POURBAIX.POLY3 TCEX40A.POLY3 (or TCEX40E.POLY3)
- copy POURBAIX.POLY3 TCEX40B.POLY3
- copy POURBAIX.POLY3 TCEX40C.POLY3
- copy POURBAIX.POLY3 TCEX40D.POLY3

or inside TCCS (under Windows NT/2000/XP, but not Windows 95/98/ME):

- @copy POURBAIX.POLY3 TCEX40A.POLY3 (or TCEX40E.POLY3)
- @copy POURBAIX.POLY3 TCEX40B.POLY3
- @copy POURBAIX.POLY3 TCEX40C.POLY3
- @copy POURBAIX.POLY3 TCEX40D.POLY3

Under Linux/UNIX platforms (outside TCCS):

- cp POURBAIX.poly3 TCEX40A.poly3 (or TCEX40E.poly3)
- cp POURBAIX.poly3 TCEX40B.poly3
- cp POURBAIX.poly3 TCEX40C.poly3
- cp POURBAIX.poly3 TCEX40D.poly3

Example TCEX40

- Using PAQ2 or PAQS2 database;
- For the Fe-H2O-NaCl heterogeneous interaction systems
- With the Main Option 1
- Using the Single-Database Option, i.e., retrieving data from the PAQ2 [TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model] or PAQS2 [TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model]; both of which contain an AQUEOUS solution phase and REF_ ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. The PAQ2 and PAQS2 are specially designed for demonstrations of calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of phase diagrams or property diagrams in some aqueous-bearing multicomponent heterogeneous interaction systems within the limited chemical framework of Fe-Co-Cr-Ni-C-N-S-H2O-NaCl, via the Single-Database Option in the advanced POURBAIX module or through the normal TDB-GES-PLOY-POST routine.

To further run the following Main Options:

- Main Option 2 for plotting many other property diagrams of the calculated interaction system;
- Main Option 3 for making another POURBAIX calculation of the same chemical system but under a different P-T-X condition;
- Main Option 4 for making a POLY3 STEPPING calculation of the same chemical system but varied with only one independent variable;

** The Main Options 2, 3 and 4 are not illustrated in this TCEX40 example.

Five more examples (TCEX40A, TCEX40B, TCEX40C, TCEX40D and TCEX40E) are also provided to demonstrate various options and features in the POURBAIX module and to show more advanced applications of the TCAQ2 and AQS2 aqueous solution databases [in the Multiple-Database Option, i.e., with appended data from the SSOL5 and SSUB5 databases].

Example TCEX40A

- Option 1
- Using the Single-Database Option, i.e., retrieving data from the PAQ2 [TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model] or PAQS2 [TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model]; both of which contain an AQUEOUS solution phase and REF_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. The PAQ2 and PAQS2 are specially designed for calculations of the so-called Pourbaix diagrams (i.e., Eh-pH plots) and other types of diagrams in aqueous-bearing multicomponent heterogeneous interaction systems, via the Single-Database Option in the POURBAIX module or through the normal TDB-GES-PLOY-POST routine.
- A POLY3 file called POURBAIX.POLY3 is automatically saved.
- For the purposes of recalling this file in other Main Options (as in the TCEX40B, TCEX40C & TCEX40D), the POURBAIX.POLY3 has to be renamed or copied as another file name (in this particular example, as TCEX40A.POLY3, and TCEX40B.POLY3, TCEX40C.POLY3 & TCEX40D.POLY3). Note that the renaming or copying has to be done outside TCCS, otherwise the POLY3 file structure will be destroyed. However, under WindowsNT/2000/XP environments, one can use MS-DOS commands to do so, e.g., @copy POURBAIX.POLY3 TCEX40B.POLY3
- The Main Option 1 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

Example TCEX40B

- Demonstration of the Main Option 2 Graphical Processing (by plotting more diagrams); various options for refining a plotted diagram (including direct interactions with the POST Module); Graphical processing of related property diagrams.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40B.POLY3), and then plotting some property diagrams for the previously calculated system.

- The loaded POLY3 file will not be modified by this Main Option. It is thus not necessary to save the file in another name; however, it is still recommended that the user to copy the TCEX40A.POLY3 (or TCEX40E.POLY3) as TCEX40B.POLY3 before the Main Option 2 is executed in this particular example.

Example TCEX40C

- Demonstration of the Main Option 3 Calculation (by modifying T-P-X conditions); graphical processing of a Pourbaix diagram.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40C.POLY3), and then making another POURBAIX-type calculation and graphical processing of a new Pourbaix diagram for the same chemical system but under a different P-T-X condition.
- The loaded POLY3 file will be rewritten according to the T-P-X settings in the new POURBAIX-type calculation. It is thus recommended to save the file in a new name outside of TCCS before this Main Option is proceeded (in this particular example, the TCEX40A.POLY3 is copied to TCEX40C.POLY3).
- The Main Option 3 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

Example TCEX40D

- Demonstration of the Main Option 4 Calculation (by utilizing various stepping variables); graphical processing of related property diagrams.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40D.POLY3), and then making some normal POLY3 STEPPING CALCULATIONs.
- The loaded POLY3 file will be rewritten according to the T-P-X and stepping variable settings in the stepping calculation. It is thus recommended to save the file in a new file name outside of TCCS before this Main Option is proceeded (in this particular example, the TCEX40A.POLY3 is copied to TCEX40D.POLY3).
- The resulting POLY3 file (in this example, TCEX40D.POLY3) can be subsequently called by a Main Option 2 for plotting more property diagrams, or by another Main Option 4 for making other stepping calculations.
- The Main Option 4 also provides the opportunity to plot many property diagrams after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

- Exploration of the possibility of modifying the definitions for some desired system-components, through the direct and internal POURBAIX-POLY3 intersection, for a STEPPING (and/or MAPPING) calculation inside the POURBAIX Module.

Example TCEX40E

- Demonstration of the Main Option 1 Calculation with the Multiple-Database Option; graphical processing of a Pourbaix diagram.

  For a more complex application than in Example 40A.

  This example requires licenses to three types of commercial Thermo-Calc databases otherwise it cannot be run, i.e.,

  - A: TCAQ2 (TCS Aqueous Solution Database, v2.5; SIT model) or AQS2 (TGG Aqueous Solution Database, v2.5; HKF model);
  - B: SSUB4 (SGTE Pure Substances Database, v4) or TCMP2 (TCS Materials Processing Database, v2);
  - C: SSOL4 (SGTE Alloy Solutions Database, v4) or TCFE6 (TCS Steels/Fe-Alloys Database, v6) or ALIKE.

- This particular example uses the multiple-database combination of TCAQ2+SSUB4+SSOL4; among them, TCAQ2 database contains only an AQUEOUS solution phase (using the SIT model) and REF_ELECTRODE phase (as a reference state for electron in aqueous electrolyte systems), SSUB4 database is appended for the GASeous mixture phase and some pure solid phases (so-called secondary phases formed during aqueous-involving interaction processes), and SSOL database is also appended for various solid solution phases.
- A POLY3 file called POURBAIX.POLY3 is automatically saved. By reading this POURBAIX.POLY3 file (or renamed as another name), one can further run the following Main Options: Main Option 2 for plotting many other property diagrams of the calculated interaction system; Main Option 3 for making another POURBAIX calculation of the same chemical system but under a different P-T-X condition; Main Option 4 for making a POLY3 STEPPING calculation of the same chemical system but varied with only one independent variable; The Main Options 2, 3 and 4 are illustrated in the TCEX40B, TCEX40C and TCEX40D examples.
- For the purposes of recalling this file in other Main Options (as in the TCEX40B, TCEX40C & TCEX40D), the POURBAIX.POLY3 has to be renamed or copied as another file name (in this particular example, as TCEX40A.POLY3, and TCEX40B.POLY3, TCEX40C.POLY3 & TCEX40D.POLY3). Note that the renaming or copying has to be done outside TCCS, otherwise the POLY3 file structure will be destroyed. However, under Windows environments,

one can use MS-DOS commands to do so, e.g., @copy POURBAIX.POLY3 TCEX40B.POLY3

- The Main Option 1 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).
- The POURBAIX module inside the TCCS software also accepts the AQS2 aqueous solution database (using the complete Revised HKF model) in the Multiple-Database Option, in addition to the TCAQ2 aqueous solution database (using the SIT model).

Example TCEX53

- Using PAQ2 or PAQS2 database; for the Fe-X-H2O-NaCl heterogeneous interaction systems (X = Cr-Ni-Co)

Note: The PAQ2 (TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model) or PAQS2 (TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model) contains an AQUEOUS solution phase and REF_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. Therefore, it can be used, via the Single-Database Option in the POURBAIX module or through the normal TDB-GES-PLOY-POST routine, for calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of diagrams in aqueous-bearing multicomponent heterogeneous interaction systems.

Note: The initial bulk composition of Fe-based alloy in this demonstrating calculation is just preliminarily assigned, in which the BCC_A2 and/or FCC_A1 solution phase(s) are considered as of primarily interest. For practical calculations, one shall have more precise inputs for the initial bulk compositions of alloys.

Console Mode TAB Module

In this section:

Tabulation of Chemical Substances, Phases or Reactions

The TAB module can be used to tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. The module can tabulate thermodynamic functions of pure stoichiometric phases or solution phases at fixed composition, as well as various kinds of partial derivatives for a pure stoichiometric phase or solution phase at a given composition.

The TAB module begins by evaluating the most stable species of a substance in either a homogeneous state or in a reaction. Results are presented in a table or plotted as a graph.

Also see *Tabulating a Reaction* on the next page.

A reaction tabulation presents you with the following properties, on rows representing different temperature levels:

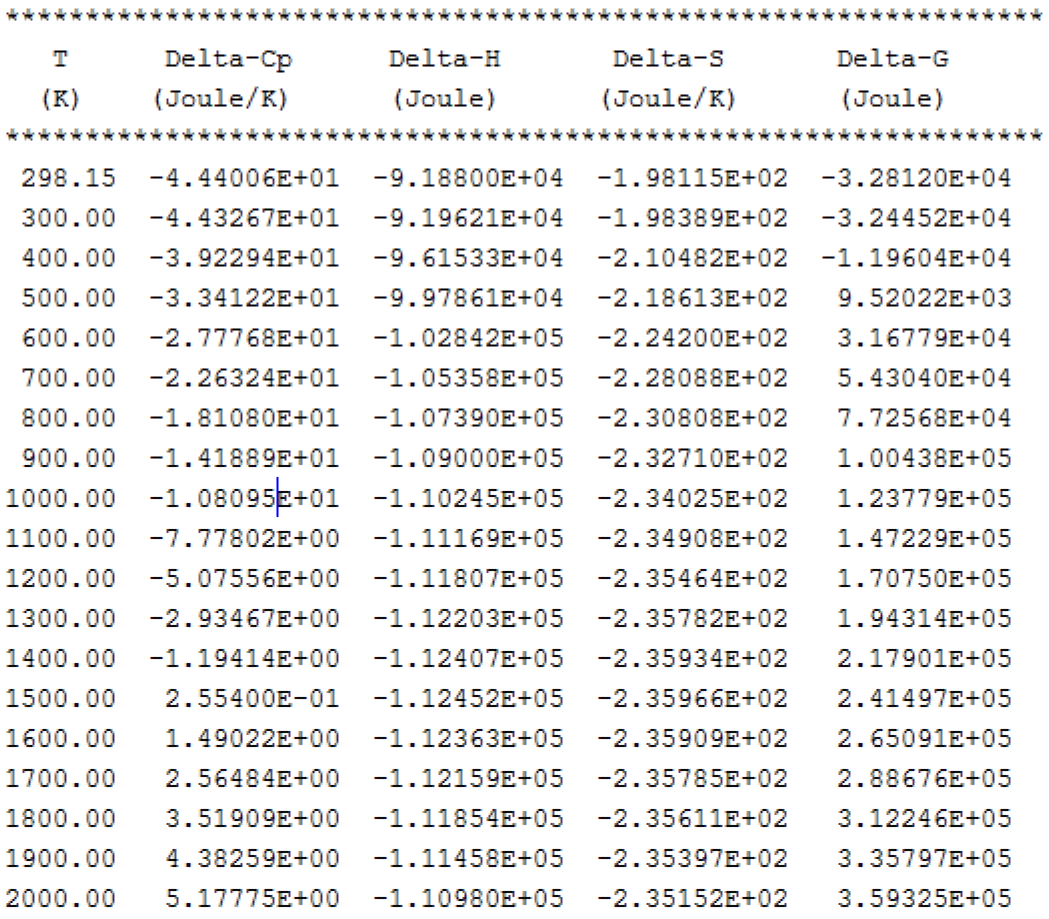
- Heat capacity change / Delta-Cp (Joule/K) in column 2.
- Enthalpy change / Delta-H (Joule) in column 3.
- Entropy change / Delta-S (Joule/K) in column 4.
- Gibbs energy change / Delta-G (Joule) in column 5.

In the case of a tabulation of a substance or solution phase at a fixed composition, the properties presented are the heat capacity, enthalpy, entropy and Gibbs energy, rather than the degree of change in those properties.

Also see *Tabulating a Substance or Solution Phase at Fixed Composition* on page 179.

You can add a 6th column to the table that shows the values of a property or user-defined function of your choice.

Reaction Tabulation Example



```
*******************************************************************
   T      Delta-Cp      Delta-H       Delta-S       Delta-G
  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
*******************************************************************
 298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04
 300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04
 400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04
 500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03
 600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04
 700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04
 800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02   7.72568E+04
 900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05
1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05
1100.00  -7.77802E+00  -1.11169E+05  -2.34908E+02   1.47229E+05
1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05
1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05
1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05
1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05
1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05
1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05
1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05
1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05
2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05
```

Tabulating a Reaction

A tabulation of a given chemical reaction provides you with data about the rate of change of the standard tabulation properties at various levels of temperature. You can also add a column for a property of your choice to the table.

TABULATION_REACTION Commands on page 247 in the *Console Mode Command Reference*.

How to Tabulate a Reaction

1. Use GOTO_MODULE TAB to enter the TAB module.
2. If you want to add one thermodynamic functions to the tabulation calculation, which is present in a sixth column in the table, use ENTER_FUNCTION.

   You are prompted to enter the name of the column that is given at its head, and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

3. Use TABULATE_REACTION followed by a formula that specifies of the reacting species and products to perform the tabulation calculation. The name of the elements must be entered in upper case letters only. Terminate the chemical reaction with a semi-colon. For example, you can enter:

   ```
   TABULATE_REACTION 3H2+N2=2N1H3;
   ```

   Elements that are designated with a single letter must be followed by a stoichiometry factor, even if this factor is 1. `CO` hence be interpreted as Cobalt rather than as carbon monoxide. Carbon monoxide is entered as `C1O1` or `O1C1`.

4. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

   The tabulation calculation is performed and you are given a table that shows the various properties at each temperature level within the range defined.

   If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column of you chose (on the Y-axis) against temperature (on the X-axis). When this graph is plotted, you are now in the POST module, where you can modify the graph in various ways.

Tabulating a Substance or Solution Phase at Fixed Composition

A tabulation of a substance or solution phase at fixed composition provides you with data about the standard tabulation properties at various levels of temperature for a given chemical reaction. You can also add one extra property column of your choice to the table.

TABULATION_REACTION Commands on page 247 in the *Console Mode Command Reference*.

How to Tabulate a Substance or Solution Phase at Fixed Composition

1. Use GOTO_MODULE TAB to enter the TAB module.
2. Use SWITCH_DATABASE to switch to a database that contains solution-based data, such as TCFE for example.

You cannot use the default SSUB database when tabulating substances or solution phases at a fixed composition.

3. If you want to add one thermodynamic function to the tabulation calculation, which is

present in a sixth column in the table, use ENTER_FUNCTION.

You are prompted to specify the column header and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

4. Use TABULATE_SUBSTANCE followed by the name of the substance or solution phase to perform the tabulation calculation.
5. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

The tabulation calculation is performed and a table shows the various properties at each temperature level within the defined range.

If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column you chose (on the Y-axis) against temperature (on the X-axis).). When this graph is plotted, you end up in the POST module, where you can modify the graph in other ways.

Console Mode POST Module

In this section:

Console Mode Visualization

The results of a calculation in Thermo-Calc can be plotted by the post-processor module, also called the POST module. The diagram is presented in the Console Results window.

In the POST module, you can define and plot various kinds of diagrams based on a calculation. You can modify diagram type, which variables to plot on each axis and between which minimum and maximum values, append experimental data from an EXP-file, change labels and symbols in the diagram, zoom in on (and out from) a certain region in a diagram, etc.

If you calculate a property or phase diagram in POLY, then you have to open the POST module yourself. If your calculation was performed by a response-driven module such as SCHEIL or POURBAIX, then the plotting of a diagram based your calculation is part of the dialogue of questions and answers you have in that module (but under the hood, the response-driven module is actually utilizing the POST module to get the plotting done).

Plotting Diagrams

Plotting a diagram is to graphically represent how several variables (typically two variables) co-vary. Each axis in a property diagram or a phase diagram represents the value of one variable. The default variables represented by the X- and Y-axes are the following:

- If you plot a diagram based on the results of a mapping operation (a phase diagram), then by default the X- and Y-axes represent the mapping axis variables 1 and 2 (set using *SET_AXIS_VARIABLE* on page 164 in POLY).
- If you plot a diagram based on the results of a stepping operation (a property diagram), then by default, the X-axis represents the stepping variable (set using SET_AXIS_VARIABLE) and the Y-axis represents the sum of the mole fractions of all phases (that is, NP(*)).

POLY_3 Commands on page 117 in the *Console Mode Command Reference*.

How to Plot a Diagram

To plot a diagram, you must have already made a stepping or mapping operation in POLY (or in some cases, made a calculation as part of some opening a response-driven module), and you must have entered the POST module.

The POST command is available inside POLY. Use POST to enter the POST module

1. If you want to directly plot your diagram with the default variables represented by the X- and Y-axes, type `Plot` and press <Enter>. This plots a property or phase diagram with the default variables represented at each axis. If you do not want to plot your diagram with these default variables, go to the next step.

2. Use SET_DIAGRAM_AXIS to set which variables to plot on the X-axis and the Y-axis. For example, if you want to plot a phase diagram with pressure on the Y-axis and temperature on the X-axis, type:

   ```
   SET_DIAGRAM_AXIS X T
   ```

   ```
   SET_DIAGRAM_AXIS Y P
   ```

3. Use PLOT_DIAGRAM to plot your diagram.

Modifying Diagrams

Modifying a diagram amounts to changing the settings that determine how the POST module presents the calculated results and plots a new diagram. Suppose that you have already plotted a binary phase diagram with the mapping axis variables temperature and mole fraction of one of your components (the Fe component, say) on the X- and Y-axes. If you then want to modify your diagram so that the Y-axis instead represents, say, the mass fraction of Fe rather than the mole fraction, then you use *SET_DIAGRAM_AXIS* on page 206 to set diagram axis `Y` to `w(Fe)`, and then use *PLOT_DIAGRAM* on page 200.

There are many ways in which you can modify your diagram and how it is presented. Any modification made in the plot settings is taken into account the next time you use PLOT.

Modification Examples

The following commands are described in the *Thermo-Calc Console Mode Command Reference*.

The following are some of the modifications you can make.

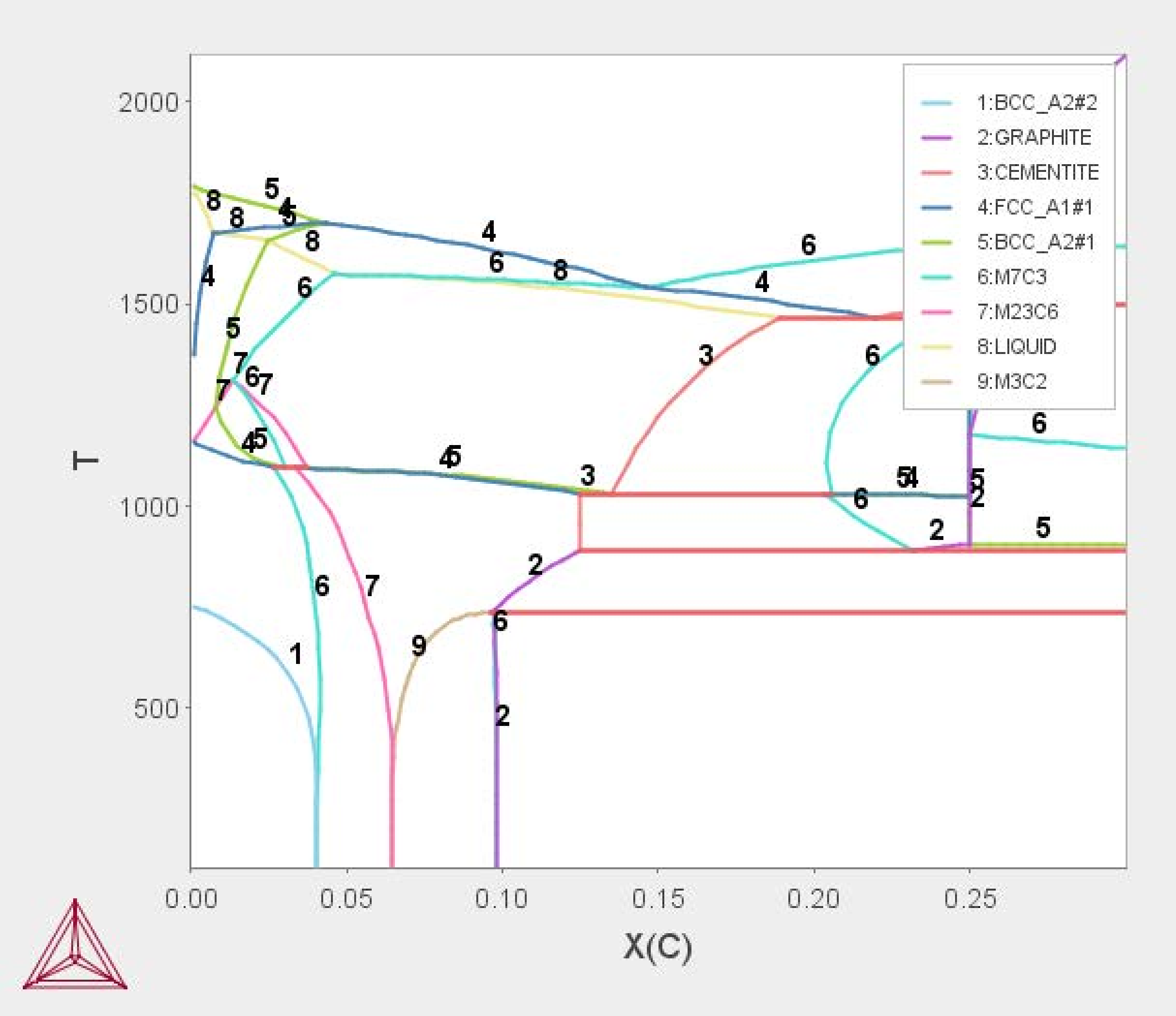
- Use *SET_TITLE* on page 215 to set add a title or to change an already existing title. The title is displayed above the plotted diagram in the Console Results window.
- Use *ADD_LABEL_TEXT* on page 190 to add a label text that starts at a certain X- and Y-coordinate. If you have plotted a phase diagram, then you can let Thermo-Calc set the label text that specifies the names of the stable phases at that coordinate.
- Use *SET_AXIS_TYPE* on page 204 to set whether the scale of an axis is linear, logarithmic or inverse.
- Use *SET_DIAGRAM_TYPE* on page 208 to plot a triangular diagram with the X-axis on the triangle’s base and the Y-axis on the triangle’s left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
- Use *SET_SCALING_STATUS* on page 214 to modify the range of values that are displayed on an axis. In effect, you can use it to zoom in or out of the diagram. For example, to set the scale of the X-axis to range from 0 to 0 .3, type:

  ```
  SET_SCALING_STATUS X N 0 0.3
  ```

The `X` specifies which axis to change the scaling on, the `N` turns off Thermo-Calc's automatic scaling, and `0` and `0.3` specifies the minimum and maximum values on the scale. You can turn on automatic scaling again by setting the second parameter to `Y`.

SET_LABEL_CURVE_OPTION Example

Use *SET_LABEL_CURVE_OPTION* on page 209 to label each set of curves that have the same stable phases with a certain digit. A legend is also added, where you specify which phases each digit designates.



LTEXT vs LaTeX Commands for Labels

As of Thermo-Calc 2015a the LTEXT text formatting is replaced by LaTeX. For existing users who may have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent:

Symbol or text format	**LTEXT**	**LaTeX**
Subscripts in an axis text	S-A-TEXT Y N Mole-fraction Al^DO2O^DO3	S-A-TEXT Y N \latex Mole-fraction Al_2O_3
Label with subscript	add .13 .15 n c-ZrO^DO2$	add .13 .15 n \latex c-ZrO_2
Greek symbol	ADD .05 .50 N ^GRd$	ADD .05 .50 N \latex \delta

Also see *Changing Global Settings* on page 189.

Saving Diagrams

When a diagram is plotted, there are several ways in which you can save it:

- Use *DUMP_DIAGRAM* on page 194 to save the diagram image to a PS, PDF, SVG, EMF, GIF, or PNG file. You are asked what format to save it in.
- To save the diagram image in a variety of image file formats, right click the diagram and select **Save Plot**.
- Use *PRINT_DIAGRAM* on page 201 to print a hard copy of the diagram.

Information about the underlying calculations that the diagram is based on is not saved in an EXP-file.

Also see the *DATAPLOT User Guide* included with this documentation set.

Loading Saved Diagrams

If you have previously saved a diagram in an EXP-file, then you can load and superimpose the diagram on another diagram. Both the following command requires you to specify which prologue and dataset(s) that are loaded from an experimental data file.

Use *APPEND_EXPERIMENTAL_DATA* on page 192 to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, the labels on the diagram are not changed when you plot the additional data from the EXP-file, irrespectively of the data in that file.

Use *QUICK_EXPERIMENTAL_PLOT* on page 201 to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, these settings are overwritten with the axes settings from the EXP-file.

About the Database Files

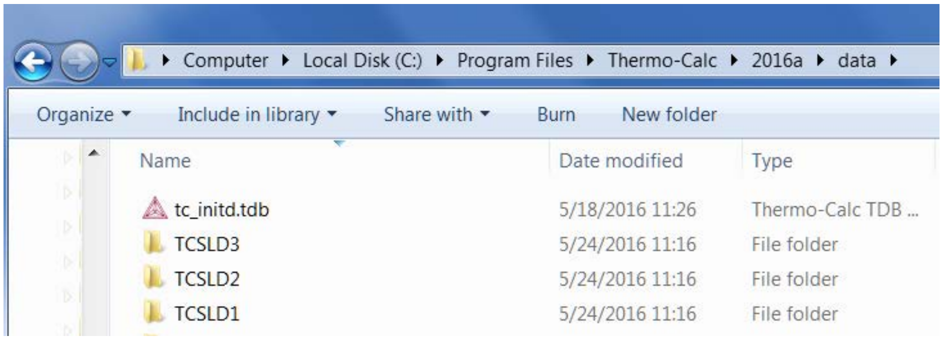
Encrypted vs Unencrypted Database Files

Any licensed databases purchased from Thermo-Calc Software are encrypted in files with the extension `.TDC`; these files cannot be edited. These are referred to as *encrypted databases*.

Unencrypted databases have the file extension `.TDB` and can be edited. For example, PURE5 or PG35 (the free databases) or a user-defined database file. If you plan to edit any of these files, see *Editing the Database Initialization File or Unencrypted Database File* on the next page for information.

Database Installation Folder

Depending on the type of license and operating system, the encrypted Thermo-Calc databases and the database initialization file are located in a subfolder to the Thermo-Calc installation. For example, in a Windows standalone installation, you can find these in a folder called **data** (file path is *C:\Program Files\Thermo-Calc\<version>\data*).



Name	Date modified	Type
tc_initd.tdb	5/18/2016 11:26	Thermo-Calc TDB ...
TCSLD3	5/24/2016 11:16	File folder
TCSLD2	5/24/2016 11:16	File folder
TCSLD1	5/24/2016 11:16	File folder

Database Initialization File

In Windows, the *database initialization file* is called `tc_initd.tdb`. In Linux and Mac it is called `initd.tdb`. The file contains a list of all the databases available from Thermo-Calc Software. Individual licenses are still required to use each database.

The file is used differently by the program depending on whether you are working with databases in Console Mode or Graphical Mode. For this reason, editing the file can be problematic if you don't understand the differences. See *About Cached Database Files (Graphical Mode only)* on the next page and *Editing the Database Initialization File or Unencrypted Database File* on the next page for more information.

User Database Files

A user-defined database is considered to be an unencrypted database because you can make changes to it.

In Graphical Mode you can add user databases via the **Options → Graphical Mode → System definer** window. Once you have added the user database it is available from the database list in the System

Definer Configuration window. See *Global Settings: System Definition (System Definer)* on page 192 to add a user database.

In Console Mode, users may decide to add their own user-defined database to the database initiation file, which then makes it available in the Console window. If you plan to edit this file, see *Editing the Database Initialization File or Unencrypted Database File* below for important information.

About Cached Database Files (Graphical Mode only)

Also see Global Settings *General* on page 190 where you can set the default database directory path.

The first time you open a database in Graphical Mode it can take a little while for it to load, especially if it is one of the large databases such as TCFE or TCNI. However, the next time the database opens quickly because now the databases are cached, or stored, in Graphical Mode.

Think of a cache as an intermediate storage area. Once a database cache is established the file made easily accessible, even if you close the software program. It is the same concept as when you load a web page for the first time. The next time the page opens faster. This is also how it works for the databases in Thermo-Calc Graphical Mode.

Thermo-Calc caches the database files, both encrypted and unencrypted types, at two points –when you first open a database, sometimes called an *in-memory cache*, and then later as a *disk-based cache*.. The disk-based cache is what speeds up database loading and it is at this point that Thermo-Calc refers to the database initialization file for information. The disk-based cache uses a lookup key to find the abbreviated database name (e.g. TCFE8 or TCNI8) contained in this initialization file.

It is important to understand the way databases are cached in Graphical Mode to ensure best practices for those who also use Console Mode, especially if the database initialization file is edited. If you plan to edit this file, see Editing a Database Initialization File or Unencrypted Database File for important information.

Editing the Database Initialization File or Unencrypted Database File

Some advanced users may decide to edit the database initialization file, for example to reorder the list of encrypted databases displaying in the Console window or to add their own user-defined database for use in Console Mode. It is important to understand that changes to this file impact the database caching process used in Graphical Mode (see *About Cached Database Files (Graphical Mode only)* above).

The following recommendations are also applicable if you edit an unencrypted database file, which includes user databases and free databases such as PURE5 or PG35.

Best Practice Recommendations

If you edit the database initialization file (tc.initd.tdb in Windows or initd.tdb in Mac and Linux), then:

- If a user database is added to the file, it is subject to the same caching as the encrypted databases. This means that further changes (to the user database) will not be detected when you are working with databases in the System Definer in Graphical Mode.

If you have a user database, which is subject to regular updates, then:

- If you make changes to a user database, you then need to clear the cache.
- It is recommended that you create a separate directory to store unencrypted database files.

If you edit an unencrypted database file included with the installation (such as the PURE5 and PG35 files):

- Do not edit the file in the installation folder. Instead make a local copy and load it into the application as a user database.

Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.

Thermo-Calc accepts deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and its add-on modules.

The executable **DatabaseChecker** file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu.

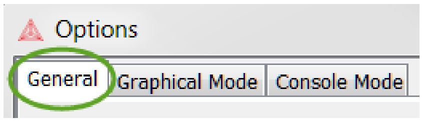
Also see the Database Manager User Guide.

Changing Global Settings

In the **Options** window (select **Tools → Options**) you can globally set general settings for Graphical Mode as well as default settings for any new activities for both Graphical Mode and Console Mode.

In this section:

General



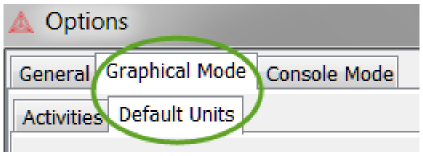
These settings are for both Graphical and Console modes. To open this window, from the main menu select **Tools** → **Options**.

General Global Settings

Setting	Options
Tooltips enabled	Select whether to turn on tooltips information. By default the **Tooltips enabled** check box is selected. This displays a small text box when you hover the cursor above some buttons or other items.
Localization	To change the GUI language from the **Localization** list choose **English** (the default), **Swedish**, **Spanish**, **German**, **Russian**, **Chinese**, **Japanese** or **French**.
Look and feel	To change the **Look and feel** of the GUI layout, choose **Windows** (the default), **Metal**, **Nimbus**, **CDE/Motif** or **WindowsClassic**.
Database directory	In the **Database directory** field, specify the path to the directory that contains the **data** directory. This is where the Thermo-Calc database directory called **data** is located. Do not specify the path to where the database files are found (that is, in the **data** directory). **Modifying the Database Directory Path (Graphical Mode Only)** Important Note: Database Directory Path (Graphical Mode only) When you open a database for the first time, it is stored in a cache (an intermediate storage area), that is maintained even if you close the program. This improves the speed of loading the next time you open that database. The cache is used for all databases that are listed in the database initialization file, typically all the standard databases that are included with Thermo-Calc. If you modify your own user-defined database, or if you choose to edit an unencrypted database, it is recommended that you create a separate directory to store these database files. This way the most recent version of the user-defined or edited databases are loaded into the program when the System Definer is performed.

Setting	Options
	⊙ Also see *About the Database Files* on page 186.
Log level	Select the level and type of information to display in the **Event Log** window using the **Log level** slide bar. Choose from a **Debug**, **Info**, **Warning** or **Error** level of detail.
Check update interval	From the **Check update interval** list, choose not to check (**Don't check**, the default) or **On startup**. You can also manually check for updates – choose **Help→Check for update**.
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Graphical Mode - Default Units



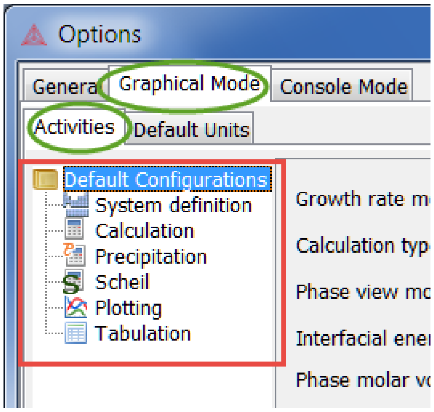
To open this window, from the main menu select **Tools → Options**and click the **Default Units** tab.

Default Units - Settings in Graphical Mode

Setting	Options
Temperature	Kelvin (the default), Celsius or Fahrenheit
Pressure	Pascal (the default), Atmospheres or Bar
Amount	Mole (the default), Gram, Kilogram or Pound
Composition	Mass percent (the default), Mole percent, Mass fraction or Mole fraction
Energy	Joule (the default), Calorie or Electron volt
Volume	Cubic meter (the default), Cubic decimeter or Cubic centimeter
Density	Kilogram per cubic meter (the default) or Gram per cubic meter
Entropy	Joules per Kelvin (the default), Calorie per Kelvin or Electron volt per Kelvin
Length	Meter (the default), Micrometer or Nanometer
Time	Seconds (the default), Hours or Days

Setting	Options
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Graphical Mode: Activities



To open this window, from the main menu select **Tools → Options** and click the **Activities** tab.

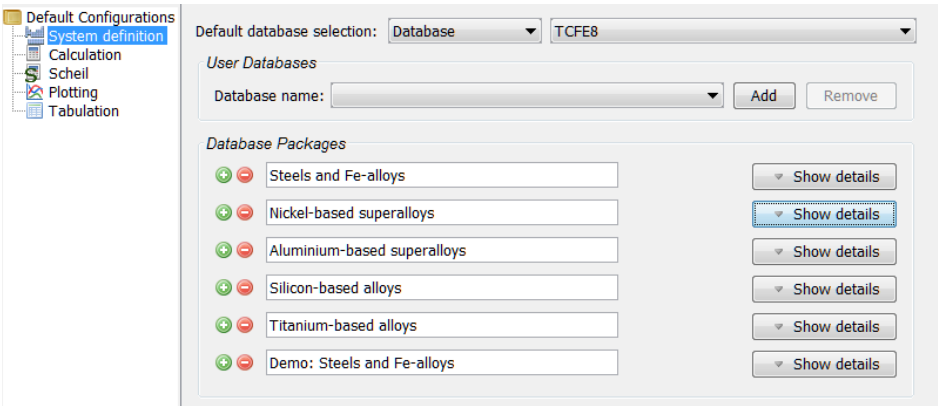
There are **System definition**, **Calculation**, **Precipitation**, **Scheil**, **Plotting** and **Tabulation** settings windows.

For Plotting, the default settings are shared with the Graphical and Console Modes. Any changes you make also apply to the default settings on the **Console Mode → Plotting** tab in the **Options** window (and vice versa). See *Global Settings: Graphical and Console Mode-Plotting* on page 202 for details.

Global Settings: System Definition (System Definer)

When you create a new System Definer, the default databases are taken from these defaults. The database selections for each System Definer can then be configured individually. Once created, the specific (local) settings for a System Definer are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **System definition**.



Default database selection: Database TCFE8

Database name:

Steels and Fe-alloys
Nickel-based superalloys
Aluminium-based superalloys
Silicon-based alloys
Titanium-based alloys
Demo: Steels and Fe-alloys

Also see *System Definer* on page 55, *Creating a Database Package* on the next page and *Clearing a Database Package Message* on page 195.

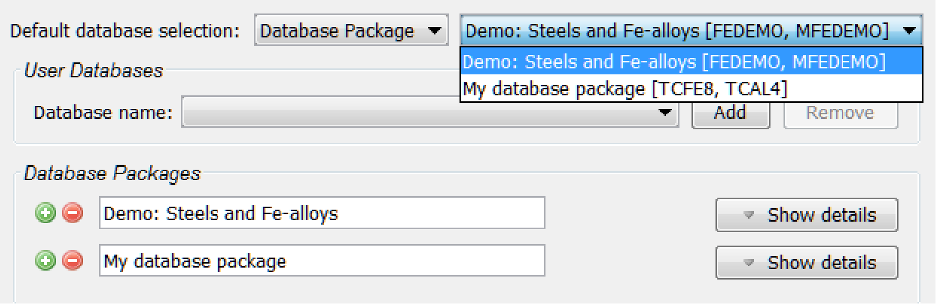
System Definer Default Settings in Graphical Mode

Setting	Options
Default database selection	Choose to define a **Database** or a **Database package**. If you choose **Database**, then select the default installed database to use globally for all System Definer nodes. For example, choose **TCFE8** or **TCNI8**. If you choose **Database Package**, select an option from the list. These Database Packages are defined in *Database Packages*.
User Databases	
Database name	Click the **Add** button to add a custom database. After you have added the user database it is available from the list to choose as the default. Once a user database is added to the **Database name** list, you can also click the **Remove** button to delete it from your project.
Database Packages	
Based on the installed databases, there are also default Database Packages available.	Create and remove **Database Packages** by clicking the **Add a database package** ⊕ button or **Remove this database package** ⊖ button. The addition or removal of a database package does not take effect until a new System Definer node is defined.

Setting	Options
	Click **Show details** to display the list of databases included with the package. Click **Hide details** to only display the name of the package. See *Creating a Database Package* below.
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Creating a Database Package

1. From the main menu select **Tools → Options** .
2. Click the **Activities** tab and click **System definition**.
3. Under **Database Packages**, click the **Add a database package** ⊕ button.
4. Replace the default text with a name for the package, for example **My database package**.
5. Select a database from the **Choose database** list, for example, **TCNI8**.
6. Click the **Add a database** ⊕ button and from the **Choose database** list, select another database, for example, **TCAL4**
7. Click **OK.** The Database Package is now available to choose as the default for new System Definer activities.

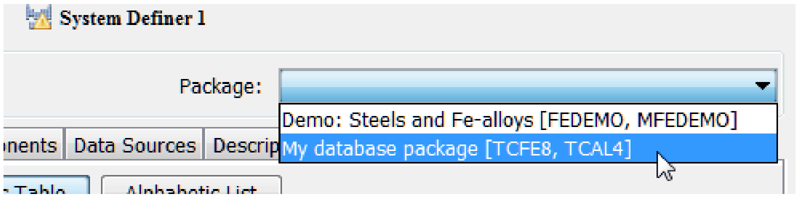


Default database selection: Database Package | Demo: Steels and Fe-alloys [FEDEMO, MFEDEMO]

Demo: Steels and Fe-alloys [FEDEMO, MFEDEMO]
My database package [TCFE8, TCAL4]

Demo: Steels and Fe-alloys
My database package

The package is available for new System Definer nodes defined after adding the package.



Package:

Demo: Steels and Fe-alloys [FEDEMO, MFEDEMO]
My database package [TCFE8, TCAL4]

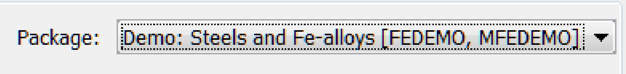
Clearing a Database Package Message below and *Global Settings: System Definition (System Definer)* on page 192.

Clearing a Database Package Message

Sometimes when working on the System Definer Configuration window, you may add or delete Databases. If you originally added a Database Package, the addition or removal of a database means that the original package you selected does not now match the databases you are using. To clear the message *Selected databases and selected package may differ* and reset the databases you need to either:

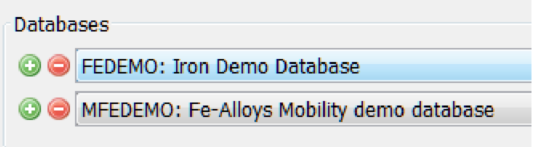
- Change the newly added database back to the one that matches the database package, or
- Choose another package from the **Package** list, then select the package you want.

For example, from the **Package** list you select **Demo: Steels and Fe-alloys**.



Package: Demo: Steels and Fe-alloys [FEDEMO, MFEDEMO]

This adds the **FEDEMO** and **MFEDEMO** databases.

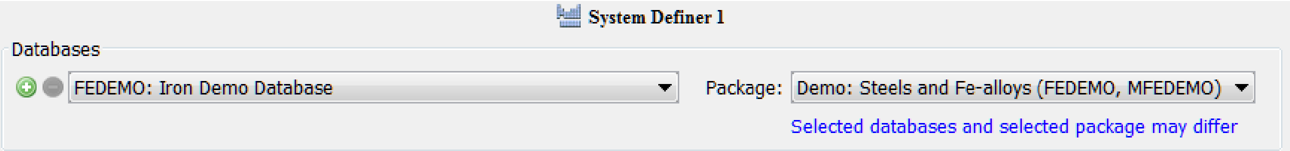


Databases

FEDEMO: Iron Demo Database

MFEDEMO: Fe-Alloys Mobility demo database

If you add or remove **Databases**, in this example **MFEDEMO** is removed, then this does not match the **Package** and the message displays:



System Definer 1

Databases

FEDEMO: Iron Demo Database

Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

Selected databases and selected package may differ

To clear the message, click the **Add a database** ⊕ button and from the **Choose database** list, select the database that belongs with the package, in this example, **MFEDEMO**. The message is cleared.

You can also choose another package from the list, which changes the databases, and then re-select the original package to reset the message.

Creating a Database Package on the previous page and *Global Settings: System Definition (System Definer)* on page 192.

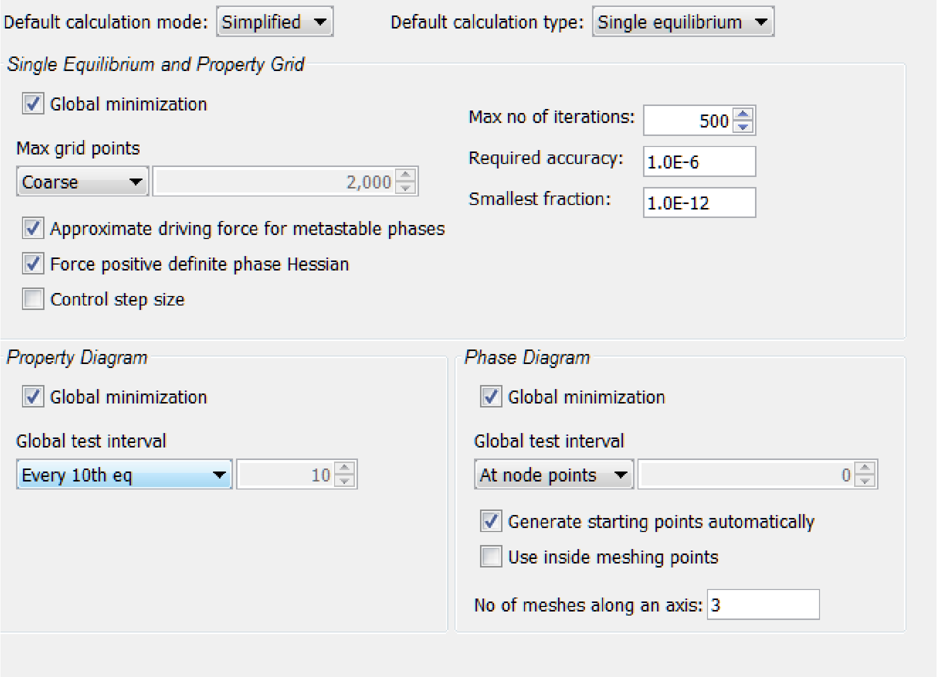
Global Settings: Calculation (Equilibrium Calculator)

When you create a new Equilibrium Calculator, its initial settings are taken from these defaults. The settings of each Equilibrium Calculator can then be configured individually. Once created, the specific (local) settings for an Equilibrium Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Calculation**.

Also see *Equilibrium Calculator* on page 73.

These settings can also be changed locally for a certain Equilibrium Calculator.



Default calculation mode: Simplified
Default calculation type: Single equilibrium

Single Equilibrium and Property Grid

☑ Global minimization
Max grid points
Coarse 2,000
☑ Approximate driving force for metastable phases
☑ Force positive definite phase Hessian
☐ Control step size
Max no of iterations: 500
Required accuracy: 1.0E-6
Smallest fraction: 1.0E-12

Property Diagram

☑ Global minimization
Global test interval
Every 10th eq 10

Phase Diagram

☑ Global minimization
Global test interval
At node points 0
☑ Generate starting points automatically
☐ Use inside meshing points
No of meshes along an axis: 3

Equilibrium Calculator Default Settings in Graphical Mode

Setting	Options
Default calculation mode	Simplified (the default) or Advanced
Default calculation type	Single equilibrium (the default), Property diagram, Phase diagram or Property grid
Single equilibrium and property grid	

Setting	Options
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Max no of iterations	By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
Max grid points	Coarse (2000 grid points, the default), Medium (20,000 grid points), Fine (200,000 grid points), or Custom (set your own number of grid points).
Required accuracy	The default is 1.0E-6. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
Smallest fraction	The default is 1.0E-12. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30. In Console Mode, the default of 1E-30 is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system.
Approximate driving force for metastable phases	The check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favourable composition and thus their driving forces may be only approximate. If it is important that these driving forces are correct, click to clear the check box to force the calculation to converge for the metastable phases.
Force positive definite phase Hessian	The check box is selected by default.
Control stepsize	The check box is selected by default
Property diagram	

Setting	Options
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Global test interval	Every 10th eq (the default), Always or Custom
Phase diagram	
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Global test interval	At node points (the default), Every 10th eq, Always or Custom
Generate starting points automatically	The check box is selected by default
Use inside meshing points	Click to select the check box as required
No of meshes along an axis	The default is 3
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Precipitation (Precipitation Calculator)

When you create a new Precipitation Calculator, its initial settings are taken from these defaults. The settings for each Precipitation Calculator can then be configured individually. Once created, the specific (local) settings for a Precipitation Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Precipitation**.

Also see *Precipitation Calculator* on page 79.

These settings can also be changed locally for a specific Precipitation Calculator.

Precipitation Calculator Default Settings in Graphical Mode

Setting	**Defaults/Options**
Growth rate model	Simplified (default) or Advanced.
Calculation Type	Isothermal (default), Non-isothermal or TTT diagram.
Phase mode view	Hide details (default) or Show details
Interfacial energy	Calculated (default) or User-defined
Phase molar volume	Database (default) or User-defined.
Matrix grain size	1.0E-4 m (default)
Matrix grain aspect ratio	1.0 (default)
Dislocation density	5.0E12 m^{-3} (default)
Nucleation sites	Bulk (default), Grain boundaries, Grain edges, Grain corners, or Dislocations.
Max time step fraction	0.1 (default)
No. of grid points over one order of magnitude in radius	150.0
Max no. of grid points over one order of magnitude in radius	200.0
Min no. of grid points over one order of magnitude in radius	100.0
Max relative volume fraction of subcritical particles allowed to dissolve in one time step	0.01
Max relative radius change	0.01
Relative radius change for avoiding class collision	0.5
Max overall volume change	0.001
Max relative change of nucleation rate in logarithmic scale	0.5
Max relative change of critical radius	0.1
Min radius for a nucleus to be	5.0E-10 m

Setting	Defaults/Options
considered as a particle	
Max time step during heating stages	1.0 s
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Scheil (Scheil Calculator)

When you create a new Scheil Calculator, its initial settings are taken from these defaults. The settings of each Scheil Calculator can then be configured individually. Once created, the specific (local) settings for a Scheil Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools** → **Options** and click the **Activities** tab. Then click **Scheil**.

Also see *Scheil Calculator* on page 109.

These settings can also be changed locally for a certain Scheil Calculator.

Scheil Calculator Default Settings in Graphical Mode

Setting	Options
Start temperature	Enter a default **Start temperature** that is higher than the liquidus temperature of the alloy, in other words, the temperature at which the alloy is completely melted.
Temperature step	Enter a default **Temperature step**. Decreasing the temperature step increases the accuracy, but the default value is usually adequate.
Global minimization	By default the **Global minimization** check box is not selected. Click to select it to perform a global minimization test when an equilibrium is reached. This costs more computer time but the calculations are more robust.
Allow BCC → FCC	By default the **Allow BCC → FCC** check box is not selected. Select the check box to allow transformations in the solidified part of the alloy caused by each of the components specified to be a *fast diffuser*. It is recommended that you only select this for steels.
Max no. of iterations	By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

Setting	Options
Required accuracy	The default is 1.0E-6. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
Smallest fraction	The default is 1.0E-12. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30. In Console Mode, the default of 1E-30 is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system.
Approximate driving force for metastable phases	The check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favourable composition and thus their driving forces may be only approximate. If it is important that these driving forces are correct, click to clear the check box to force the calculation to converge for the metastable phases.
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Tabulation (Table Renderer)

When you create a new Table Renderer, its initial settings are taken from these default settings. The settings of each Table Renderer can then be configured individually. Once created, the settings of a Table Renderer are not affected by changes in the default settings. To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Tabulation**.

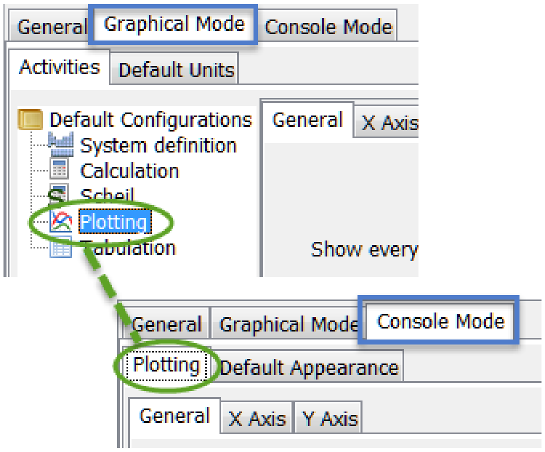
Also see *Table Renderer* on page 102.

Table Renderer Default Settings in Graphical Mode

Setting	Options
Decimal digits	The default is 5
Number format	Auto (the default), Decimal or Scientific
Phase description detail	Composition (the default), Condensed, Constitution, or Composition and constitution
Primary display color	Click **Modify** to change the default
Secondary display color	Click **Modify** to change the default
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Graphical and Console Mode-Plotting

The default settings are shared with both modes. Any changes you make also apply to the default settings on the **Console Mode → Plotting** tab in the **Options** window (and vice versa).



To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. In the **Plot Properties** window a variety of settings can be made.

You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included). In the **Results** window, hover the mouse over a plot line. The crosshair cursor turns into a cursor resembling a pointing hand when it is over a line that can clicked. Alternatively, hold down Ctrl while you move the cursor around the plot to only display it as a crosshair and prevent unintended edits.

To globally configure the default settings for plotting, from the main menu select **Tools → Options**. Click the **Graphical Mode → Activities** tabs and then click the **Plotting** node.

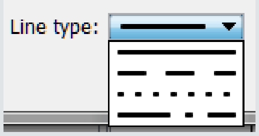
When you create a new Plot Renderer, its initial settings are taken from these default settings. The settings can then be configured individually. Once created, the settings of a Plot Renderer are not affected by changes to the default global settings.

To configure the settings of an individual Plot Renderer rather than the default settings, right-click a plot in the **Results** window and select **Properties** from the menu.

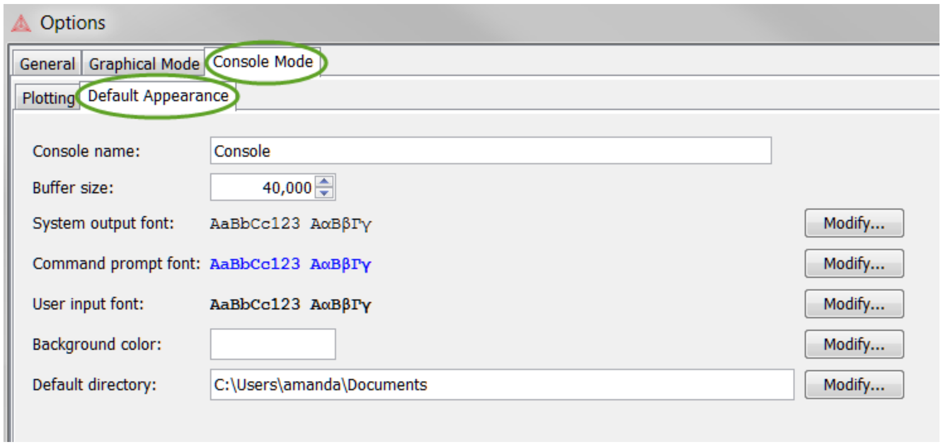
Plot Renderer Settings for Console and Graphical Modes

These global settings are available for both Console and Graphical Modes.

Setting	Options
Title	Enter a title. Select **Plain text** (the default) or **LaTeX formatted text**. Click α button to add symbols. Click a symbol category (for example, Latin characters or Greek and math symbols). Then click to choose the symbol located on the right-hand side. When you select **LaTeX formatted text** you can use the LaTeX math text to enter text. See *ADD_LABEL_TEXT* on page 190 and *Adding and Editing Plot Labels* on page 93 for more details.
Title font, Legend font, Label font, Header font	Click **Modify** to edit the Font Name, Style, Size and Color.
Legend phase caption style	Choose **All**, **Constitution description** or **Ordering description**. See *About Legend Styles* on page 92 for details about these options.
Legend background color, Background color, Canvas color, Border color,	Click **Modify** to choose a color or enter a specific color.
Label format	Select Plain text (the default) or LaTeX formatted text.
Show anchor	By default, an anchor between the label and the plot point is displayed.
Retain labels (Graphical Mode only)	By default the check box is selected. Plot labels are kept (retained) when plots are updated. It can be applied globally or locally to individual plots.

Setting	Options
Show header (Console Mode only)	Click to select the **Show header** check box to display the basic details about the plot along the top. This includes the date and time the plot is generated, the database used and the properties.
Border width	Choose a plot border width between **1** (thin, the default) and **10** (thick).
Color option	For the plot line colors, choose from the options in the list: **Legacy**, **Printer friendly**, **JFree chart**, **Pastel**, **Medium dark**, **Bright dark**, **Vivid** or **Earth**. This option is also available for specific plot lines. To change the color of an individual plot line double-click it in the Results window and use the color palette to define it or enter a specific color.
Line width	For the plot line width, choose from the options in the list. These options are also available for specific plot lines. To change an individual plot line width double-click it in the Results window.
Line type	This option is only available for individual plot lines. To change an individual plot line type double-click it in the Results window and choose an option from the list. 
Show data points	Click to select the check box to display the data points on the plot lines. This option is also available for specific plot lines. To show data points on an individual plot line double-click it in the Results window and select the check box.
Data point marker size	Choose the data point marker size between **1** (small) and **10** (large). The default is 3.
Plot area size	The **Fit the plot area size to the enclosing window** option is selected by default. Excluding triangular plots, click Define the plot area size to enter a Plot area height and Plot area width.
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Console Mode Default Appearance



Console name: Console
Buffer size: 40,000
System output font: AaBbCc123 AαBβΓγ
Command prompt font: AaBbCc123 AαBβΓγ
User input font: AaBbCc123 AαBβΓγ
Background color:
Default directory: C:\Users\amanda\Documents

To open this window, from the main menu select **Tools → Options**. To change the name, buffer size, fonts and colours for a specific Console window, right-click the label for that particular Console and select **Properties**.

Default Appearance Settings in Console Mode

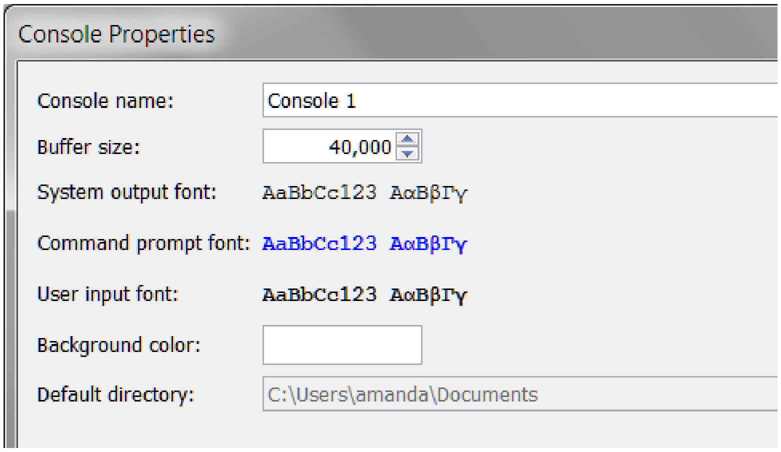
Setting	Options
Console name	The default is `Console` or enter another name to display
Buffer size	The default buffer size is 40,000.
System output font	Click **Modify** to open the **Select Font** window and makes changes to the font type, style, size or color as required.
Command prompt font	
User input font	
Background color	Click **Modify** to open the **Select Color** window to choose a background color for the Console Mode window where you enter commands.
Default directory	Set the default directory where log files and workspace files are saved.
Reset to original settings	In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Increasing the Buffer Size

Sometimes the output overflows the window text buffer (see *Controlling Console Output* on page 125). To increase the buffer size in a specific Console tab:

1. Right-click the Console tab header in the Console window (if this is the first Console tab, it is labelled **Console 1**).

2. Click **Properties**, and increase the **Buffer size** in the Console Properties window.



Console Properties

Console name: Console 1

Buffer size: 40,000

System output font: AaBbCc123 AαBβΓγ

Command prompt font: AaBbCc123 AαBβΓγ

User input font: AaBbCc123 AαBβΓγ

Background color:

Default directory: C:\Users\amanda\Documents

Console Mode Command Reference

Thermo-Calc Version 2016b

Thermo-Calc Software

Introduction to the Command Reference

In this section:

About the Console Command Reference

This command reference is for Console Mode users of Thermo-Calc software. This guide describes the function and syntax of the commands available in the Thermo-Calc modules.

If you have the Diffusion Module (DICTRA) also see the *Diffusion Module (DICTRA) Command Reference* found in the Diffusion Module (DICTRA) Documentation Set PDF.

The commands available in all or most modules are described in the first topic (*General Commands* on page 3). The next topics are listed in alphabetical order based on the module names, then in each subtopic, the module commands.

Abbreviations Used in this Guide

For the prompts, `Y` stands for Yes and `N` stands for No.

TC is for Thermo-Calc. For example, default file names often start with `tc.ini`.

File Types

Also see the *Thermo-Calc Installation Guide* and the *Data Optimization User Guide* included with this documentation set for information about EXP files.

In Console Mode, Thermo-Calc uses different kinds of files, including:

- Log files (*.LOG)
- Macro files (*.TCM or *.LOG)
- POLY workspace files (*.POLY3)
- Experimental data files (*.EXP)
- The GIBBS module uses a workspace file (*.GES5)
- The PARROT module uses files with the suffixes *.PAR and *.POP.

General Commands

In this section:

BACK

Also see *GOTO_MODULE* below.

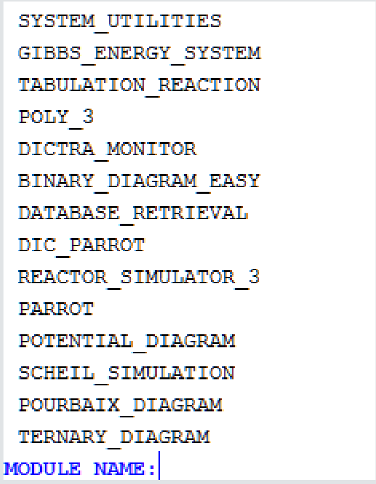
Syntax	BACK
	Switch control back to the most recent module. Going from the POST module (post-processor), BACK goes only to the TAB or POLY module (from where the POST module is entered).

EXIT

Syntax	EXIT
	Exit the program and return to the operating system. Use a save command before exiting otherwise all data and results are lost (in either the GIBBS, POLY, PARROT or REACTOR module).

GOTO_MODULE

Switch between modules. The name of the module must be typed. To get a list of available modules, press the <Enter> key.

Syntax	GOTO_MODULE
Prompt	`MODULE NAME: <MODULE NAME>`
	If the <Enter> key is pressed without typing a unique module name (or typing a ? mark) it prompts for the `MODULE NAME` and lists the available modules 

```
 SYSTEM_UTILITIES
 GIBBS_ENERGY_SYSTEM
 TABULATION_REACTION
 POLY_3
 DICTRA_MONITOR
 BINARY_DIAGRAM_EASY
 DATABASE_RETRIEVAL
 DIC_PARROT
 REACTOR_SIMULATOR_3
 PARROT
 POTENTIAL_DIAGRAM
 SCHEIL_SIMULATION
 POURBAIX_DIAGRAM
 TERNARY_DIAGRAM
MODULE NAME:
```

HELP (? and ??)

Gives text help about the current prompt (whether this is the prompt of a module, or a prompt that requests you to specify the value of some parameter).

Syntax	? OR ??
	For some commands and prompts, more detailed help is given when two ?? are entered.

HELP

Lists the available commands or explains a specified command. Specifying a unique command displays an explanation on screen. Typing a command abbreviation that is not unique lists all matching commands. Get the command information by typing a unique abbreviation or the complete command name.

Syntax	HELP
Prompt	`COMMAND: <COMMAND NAME>` *Command name* is the name of the command (one of the-module commands) to get help. If the <Enter> key is pressed without typing a command name, then all the available commands are listed.

INFORMATION

Get basic information about topics related to the module you are in.

Syntax	INFORMATION
Prompt	`WHICH SUBJECT /PURPOSE/: <TOPIC NAME>` Specify a Subject (or its abbreviation as long as it is unique). Enter a question mark ? for a list of topics.

MACRO_FILE_OPEN

The macro file functionality is a way to predefine sequences of Thermo-Calc commands stored in a macro file (a basic text file usually with the default extension TCM for the Thermo-Calc Console Mode or DCM for DICTRA module) and then executing all of the sequences using this command (preceded by the macro file name). This command can be used within various modules (i.e. the SYS, POLY, PARROT and TAB modules in the Thermo-Calc (Console Mode) software; SYS, POLY, PARROT and DICTRA_Monitor).

Syntax	MACRO_FILE_OPEN
	`<NAME OF A MACRO FILE *.TCM>` An **Open** window displays to specify the filename of the macro file (*.TCM) with the macro command, so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** *.TCM for Thermo-Calc (Console Mode) calculations and *.DCM for DICTRA simulations, cannot be changed. Click **Open** or **Cancel** to continue. If the macro file contains commands to set *.LOG files, to save or read GIBBS, POLY or PARROT workspaces, switch user databases, compile experiments (from existing *.POP files), create new *.PAR files, append *.EXP files, plot or dump diagrams, etc., a window (e.g. Save, Open, Print, etc.) displays on screen. If required, these windows can be avoided by issuing the file names (preferably with file-type extensions; if the files are not in the current working area where the macro is located, the appropriate and complete paths of the files should also be specified) and sometimes with the required options after the corresponding commands or parameters/options. For details, see the related commands and modules. When using a macro file that intended to plot graphs on screen, but the command *SET_PLOT_FORMAT* on page 210 is used to alter the plotting environment from the default value, it is important to first use the command SET_PLOT_FORMAT again to change back to the default value.

See example 12 in the *Console Mode Examples Guide*.

This is useful when the same or similar calculations are made frequently with small changes [in terms of system definitions, data manipulations, conditions (for single points, stepping or mapping calculations), plotting settings, etc.). For example, use this feature when calculating phase/property diagrams during an assessment of thermodynamic data.

A macro file can be automatically generated by the Thermo-Calc (Console Mode) software, if in the SYS module the *SET_LOG_FILE* on page 244 command is used and a *.LOG file name is given before any other SYS, DATA, TAB, GIBBS, POLY, POST, PARROT, or ED-EXP command or any special-module command (e.g. BIN, TERN, POTENTIAL, SCHEIL, POURBAIX, or REACTION). Such a *.LOG file generated from the Thermo-Calc (Console Mode) software is a textual file, and using a textual editor (such as Notepad, WordPad, PFE, Emacs, vi, etc.) it can be edited, for example, by taking away unnecessary command lines, modifying some commands, settings and definitions, adding some pausing points, adding helpful commenting lines beginning with @@ signs, and so forth. Then save it as a macro file with the standard file extension TCM.

Experienced users can also write/edit an appropriate macro file for calculations/simulations, using any basic textual editor outside the Thermo-Calc program.

All commands can be used in a macro file. The file must be terminated with EXIT or be interrupted with SET_INTERACTIVE.

Within a macro file you can use comment-lines (for describing the problems and for explaining commands and inputs/outputs), which should always start with the @@ signs in the beginning of each comment-line. Such comment-lines help to document the macro file, while these are not considered as command lines and thus do not affect the proceeding of all the normal commands in modules of the Console Mode when the file is called by the Thermo-Calc Console Mode software.

You can put multiple-line comment-blocks in a macro file between the @ (” and “@)” signs. The former sign indicates where the comment begins and the latter sign indicates where the comment ends. A comment-block begins from a line started with the *begin comment* sign @ (and ends with the *finish comment* sign @); all the lines written in between are ignored, and the line started with @) is also ignored.

Another use for a macro file is to allow you to interact at some specific points, using the “@?” sign starting a text line (note that the text describing the expected user-specification/input should be written as a continuous string without any empty space), for user’s on-time specifications of arguments/parameters or inputs of parameter-values that are requested by a certain command. The macro temporally stops at the “@?” sign, prompt on screen the text given after “@?”, and waits for the specified argument/parameter/value. The Thermo-Calc (Console Mode) software then uses specified argument/parameter/value as the input(s) for the associated command. For example, you can input the values of lower and higher temperature limits for the second axis-variable as follows:

```
GO POLY-3
SET-AXIS-VAR 2 T  @?Low-temperature-limit:
@?High-temperature-limit:
```

You can have macro-variables denoted by the signs of @#n (for definition) and ##n (for usage); and up to nine variables inside a single macro file. Such a macro-variable can be assigned with its desired value, as for example:

```
@#3First-element?
```

This writes the text (note that the text describing the expected user specification/input is written as a continuous string without any empty spaces) after the “@#3” sign as prompted on screen and then wait for a specification. The input is assigned to the macro-variable ##3, which is directly called in different parts within the current macro file.

For example, the content of the macro-variable `##3` is inserted in the command:

```
DEFINE-SYSTEM ##3
```

It is also useful in more complicated commands, such as:

```
SET AXIS VAR 1 x(##3) 0 1,,,
```

This command sets the mole fraction of macro variable 3 as axis 1.

A macro file can have any number of pauses at the `@&` signs, for the purpose of checking the details/results of executing certain commands when running the macro file. However, you can also prevent the Thermo-Calc (Console Mode) software from temporarily stopping at any pause by typing any character (except for the `Y` character for confirming a Yes answer to a command prompt) after specifying the name of a macro file.

A macro file can have a maximum of five nested levels, i.e. a macro file can call another macro file, and if one sub-level macro is terminated by the command it resumes at the next command in the previous macro. If it is terminated by `end-of-file`, the Thermo-Calc (Console Mode) software stops.

This feature is especially useful for alloy design that requires many (hundreds) of calculations/simulations on similar material system/processes (specified in many different but appropriately-documented macro files that are organized in up to five levels) during a certain period of time (e.g. in an evening), you can run the main macro (on the top level) at a certain time (e.g. before leaving the office) and afterwards (e.g. next morning) you can systematically and efficiently check/compare/analyse the results (saved as graphical files, and/or EXP, TXT, XLS… files).

By adding the SYS command *SET_ECHO* on page 244 at the beginning of a macro file (or in the primary macro file on the top level if any sub-level(s) of macro files are used), it is useful to automatically display the complete/detailed meaning of various commands in all the sequential operations in the software, all enforced according to the macro file(s).

SET_INTERACTIVE

Syntax	SET_INTERACTIVE
	Resets the input and output units to the initial values, i.e. keyboard and screen. Add this as the last command to the macro files.

BINARY_DIAGRAM Commands

In this section:

BINARY_DIAGRAM Module

The BINARY_DIAGRAM module (short name, the BIN module) enables you to quickly calculate a simple binary phase diagram. Access to specific databases designed for BIN, such as TCBIN, is required.

To enter the module, at the SYS prompt type `GOTO_MODULE BINARY`. There are no other commands for this module. Follow the prompts to plot a diagram.

Also see the Graphical Mode equivalent to this command, *Binary Calculator* on page 105 in the *Thermo-Calc User Guide*.

Syntax	BINARY_DIAGRAM
Prompts	`DATABASE: /TCBIN/`
	`FIRST ELEMENT` `SECOND ELEMENT`
	`PHASE DIAGRAM, PHASE FRACTION (F), G- OR A-CURVES (G/A): /PHASE_DIAGRAM/`

DATABASE_RETRIEVAL Commands

Search the online help or see in the *Thermo-Calc User Guide* for step-by-step instructions to define a system.

In this section:

AMEND_SELECTION

Use this command after defining the elements, species or the system (with the commands *DEFINE_ELEMENTS* on page 14, *DEFINE_SPECIES* on page 14, or *DEFINE_SYSTEM* on page 15). The prompts allow changes to the predefined system. By answering Y or N, each of the selected elements, species or phases can be accepted or rejected (although this is not the case for the constituents or the entire system).

Syntax	AMEND_SELECTION
Prompt	`KEEP <NAME1> NO/QUIT /YES/` `KEEP <NAME2> NO/QUIT /YES/`
Options	`KEYWORD-- ELEMENTS/SPECIES/PHASES NAME&` Names of the pre-defined or pre-selected elements/species/phases

APPEND_DATABASE

Append data from a file or additional database to the current set of data already read from another database. Data already read from another database and stored in the Gibbs energy system is kept in the GES5 workspace.

This command also enters all additional parameters (phase constituents, G0 and interaction parameters, etc.) to already existing phases, and all existing parameters (phase constituents, excess model, G0 and interaction parameters, etc.) in the phase are replaced with the values retrieved from the appending database.

The command is equivalent to the SWITCH_DATABASE USER command sequence. It is also similar to *SWITCH_DATABASE* on page 20, but does not reinitialize the DATA module and GIBBS workspace.

All the directly connected databases as predefined by the original database initiation file (TC_INITD.TDB file in the /DATA/ area for Windows environments, or the `initd.tdb` file in the \data\ area for Linux), or by a user-specified database initiation file after using *NEW_DIRECTORY_FILE* on page 17, are listed after pressing <Enter> without giving any argument. You can supply your own database by giving the argument `USER`, the database name and the correct path if it is not located in the current working directory.

After the command is executed for the first time, the TDB_XYZ: prompt (XYZ stands for the name of the primary switched database) is changed to the APP: prompt to go to more commands related to appending data.

Syntax	APPEND_DATABASE

Prompt	Use one of these databases
	`PURE   = SGTE PURE ELEMENT DATABASE`
	`SSUB   = SGTE SUBSTANCE DATABASE 1997`
	`USER    = USER DEFINED DATABASE`
	`DATABASE NAME /XYZ/: <ADDITIONAL DATABASE NAME>`

Options	`ADDITIONAL DATABASE NAME` The name of an existing database or a USER database definition file (***setup.TDB) that corresponds to the appending database.
Notes	If a USER database name or its path is not given on the same line of the APPEND_DATABASE command, or if the name or path is incomplete or incorrect, an Open window displays to open an appropriate database-setup. You can then open the USER database, or can cancel the open session; in the latter case, the program lists all predefined databases in the installation area, and you can select one of these or proceed with the USER option again for appending a desired database. When this command is used in a macro (*.TCM) file, if the USER option is selected, the database setup file name (*setup.TDB) containing the setup definitions of the USER database, and its correct path, are required. In Linux, the filename of a USER database, or one of the predefined names, can be used under the prompt `FILENAME`: This is a valid filename for the USER database definition file (***setup.tdb) or a predefined database name, with the correct path. The default filename extension is *.tdb*. This command can be called more than once if appending two or more databases to the primary switched database. After this command, the commands to define a system (in terms of either elements or species), to reject/restore phases or species, and retrieve data must be repeated; however, the second keywords and parameter values might have to be different from the previous ones.

DATABASE_INFORMATION

Syntax	DATABASE_INFORMATION
	A short description of the current database is normally given by typing this command. This can include information on covered systems, used models, valid ranges for parameters in temperature and composition, major applications, and so on.

DEFINE_ELEMENTS

Define the system in terms of elements. All possible species that can be formed by the given elements are retrieved from the database. The names of elements must be separated with a space or comma. It is possible to use a wildcard * after a common part of element names so that all the elements, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 40 elements can be defined into a single system.

Also see *Defining a System in Console Mode* on page 129 in the *Thermo-Calc User Guide* for step-by-step instructions to define a system with this command.

Syntax	DEFINE_ELEMENTS
Prompt	`ELEMENT& <ELEMENT1, ELEMENT2, …>` A list of elements to be defined into the system.
	When appending database(s), this command, or *DEFINE_SPECIES* below or *DEFINE_SYSTEM* on the next page must be repeated with the same or similar elements as defined in the first switched database.

DEFINE_SPECIES

Define the system in terms of species. Only those species given are retrieved. The different names of species must be separated with a space or comma. It is possible to use a wildcard * after a common part of species names so that all the species, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 1000 species can be defined in a single system.

Also see *Defining a System in Console Mode* on page 129 in the *Thermo-Calc User Guide*.

Syntax	DEFINE_SPECIES
Prompt	`SPECIES& <SPECIES1, SPECIES2, …>` A list of species to be defined in the system.
	When appending database(s), this command, *DEFINE_ELEMENTS* above or *DEFINE_SYSTEM* on the next page must be repeated with the same or similar elements as defined in the first switched database.

DEFINE_SYSTEM

Define the system in terms of either elements (equivalent to *DEFINE_ELEMENTS* on the previous page) or species (equivalent to *DEFINE_SPECIES* on the previous page). Certain databases have a default value of the keyword (as either ELEMENTS or SPECIES) reflecting what is most appropriate when defining a system.

The different names of elements or species must be separated with a space or comma. It is possible to use a wildcard * after a common part of elements or species names so that all the elements or species, which start with that common part and are available in the currently switched or appending database, are defined in the system.

When appending database(s), this command (or DEFINE_ELEMENTS or DEFINE_SPECIES) must be repeated with the same or similar elements as defined in the first switched database. Different databases might contain different elements and have different species definitions: avoid defining elements/species that are missing in the appending database(s). Otherwise, the program indicates these missing elements/species, and ignores them in subsequent steps. But additional elements/species, and additional phases not available in the first switched database can be defined and retrieved from the appending database(s). Up to 40 elements and 1000 species can be defined in a single system.

Also see *Defining a System in Console Mode* on page 129 in the *Thermo-Calc User Guide* for step-by-step instructions to define a system with this command.

Syntax	DEFINE_SYSTEM
Prompt	`ELEMENTS: <ELEMENT1, ELEMENT2, …>, OR` `SPECIES: <SPECIES1, SPECIES2, …>`
Options	**Description**
`SPECIES OR ELEMENTS`	Default keyword.
`ELEMENT&`	Specify a list of elements for the defining system.
`SPECIES&`	Specify a list of species for the defining system.

GET_DATA

Only after executing this command can you go to any of the application programs such as GES, POLY or DICTRA and use the retrieved data. When appending database(s), this command must be repeated in order to obtain the additional system definitions, parameters and functions.

Syntax	GET_DATA
	Enter the defined system's elements, species, phases, and the connected parameters obtained from either the primary switched or additionally appending database(s) to the GIBBS and/or DICTRA workspace. This command is necessary for retrieval of all information concerning a defined system from the databank.

LIST_DATABASE

List all elements, species, phases or phase constituents in the database.

Syntax	LIST_DATABASE
Options	**Description**
`KEYWORD`	One of the keywords Elements, Species, Phases or Constituent must be used to indicate what to list
`ELEMENTS`	All available elements, the reference state, atomic mass, H298-H0 and S298. Some elements have spaces in the column for the reference state. This implies that there are no parameters stored for this element.
`SPECIES`	All available species together with the stoichiometric factors.
`PHASES`	All available phases together with the number of sublattices and the number of sites in each sublattice.
`CONSTITUENT`	All available phases, the number of sublattices, the number of sites in each sublattice and the species dissolved in each phase. Species in different sublattices are separated with a colon (:). It is important to realize, for example, a phase can consist of Fe, Mo, V, and Cr, and its thermodynamic parameters can come from the binary systems Fe-Mo, Fe-V, Fe-Cr, and Mo-Cr. These data can give a relatively good description of the corners of the Fe-Cr-Mo system, but would most certainly give a bad one for the system Mo-Cr-V, due to the fact that the interaction parameters are, by default, set to zero, which originates from binary systems not included in the database.

LIST_SYSTEM

List all elements, species, phases or phase constituents in the defined system. It works only after a system is defined.

Syntax	LIST_SYSTEM
Keyword	One of the keywords `Elements`, `Species`, `Phases` or `Constituent` (as described in *LIST_DATABASE* above) must be used to indicate what to list.

NEW_DIRECTORY_FILE

Open a new database initiation file (or called database directory file) generated by a local database manager or user, for accessing additional databases not predefined in the original database initiation file.

The original database initiation file is automatically copied by the installation script to the main database area, on a local computer for an independent installation locates or a connected server for a server installation.

- For Windows this is the TC_INITD (or TC_INITD.TDB) file in the \DATA\ area under the directory defined by the TCPATH parameter.
- For Linux, it is the initd.tdb file in /data/ area that is under the directory defined by the TC_DATA parameter. If the Thermo-Calc (Console Mode) is run on a Linux platform, the new database initiation file must be located in the current working directory.

If there are too many databases at one installation or if there are some user-specified databases for a particular purpose, a local database manager can generate additional database initiation files, or each user can have their own initiation file.

The command switches the working initialization of database groups in the DATA module among the original and additional database initiation files. The Thermo-Calc (Console Mode) can use additional database initiation files that define accessing paths to database groups (databases located in different subdirectories under the directory defined by the TCPATH or TC_DATA parameter). All directly accessible databases remain as in the same group, until this command is called or recalled.

Syntax	NEW_DIRECTORY_FILE

Prompt	`FILE WITH DATABASE DIRECTORY /TC_INITD/: <DATABASE-INITIATION-FILE NAME>`
	`ANOTHER DATABASE-INITIATION-FILE NAME`
	The name of the next database initiation file (either additional or original) that is to be switched on as follows sessions.

	✎ If the file name or its path is not given on the same line of the NEW_DIRECTORY_FILE command, or if it is incomplete or incorrect, an **Open** window displays to specify the new database initiation file.

REJECT

Reject elements, species, phases or phase constituents that can form from the defined elements and species. Phases/species/constituents that are possible to form in the defined system are removed from the list of system phases/species/constituents (shown by the command *LIST_SYSTEM* on the previous page). Phases/species/constituents that are not included in the list cannot be entered without first being restored. The different names must be separated with a space or comma. You can use a wildcard * after a common part of names so that all the elements/species/phases/constituents that start with that common part and are available in the currently switched or appending database, are rejected from the defined system.

This command can also reject a defined system, and thus reinitiate the entire DATA module memory and GES5 workspace.

Syntax	REJECT
Prompt 1	(keyword = ELEMENTS or SPECIES or PHASES) `IF KEYWORD: <NAME1, NAME2, …>`

Prompt 2	(if keyword = CONSTITUENT)
	`PHASE: <PHASE NAME>`
	`SUBLATTICE NUMBER: <SUBLATTICE NUMBER IN THE PHASE>`
	`CONSTITUENT: <CONSTITUENT(S) IN THE SUBLATTICE OF THE PHASE>`

Prompt 3	If keyword = SYSTEM the DATA module is reset to its initial state; GIBBS is reinitiated and data already entered to GES5 is lost.
Options	**Description and additional information**
`KEYWORD`	One of the keywords `Elements`, `Species`, `Phases`, `Constituent` or `System` must be used to indicate what is rejected.
`NAME&`	Names of the pre-defined elements/species/phases/constituents/system
`ELEMENTS`	The given elements are rejected.
`SPECIES`	The given species are rejected, making it impossible to form them from the defined elements.
`PHASES`	The given phases are rejected, making it impossible to form them from the defined elements or species.
`CONSTITUENT`	The given constituent in one phase are rejected. Add the following when prompted: `Phase`: The name of the phase containing the constituent to be rejected. `Sublattice number`: The sublattice where the constituent enters (the first sublattice is 1). The question is omitted if there exists only one possible sublattice. `Constituent`: The name(s) of the constituent(s) to be rejected.

RESTORE

Restore already explicitly rejected elements, species, phases or constituents; it is the opposite of the command *REJECT* on the previous page although it does not restore a completely rejected system.

Phases/species/constituents that are possible to form from the defined elements or species are entered to the list of system phases/species/constituents (shown by the command *LIST_SYSTEM* on page 16). Phases/species/constituents that are not included on the list can now be added to the list. The different names must be separated with a space or comma. It is possible to use a wildcard * after a common part of names so that all the elements/species/phases/constituents, which start with that common part and are available in the currently switched or appending database, are restored in the defined system.

Syntax	RESTORE
Prompt1	(if keyword = ELEMENTS or SPECIES or PHASES) `KEYWORD: <NAME1, NAME2, …>`

Prompt2	(if keyword = CONSTITUENT)
	`PHASE: <PHASE NAME>`
	`SUBLATTICE NUMBER: <SUBLATTICE NUMBER IN THE PHASE>`
	`CONSTITUENT: <CONSTITUENT(S) IN THE SUBLATTICE OF THE PHASE>`

Options	**Description and Information**
`KEYWORD`	One of the keywords `Elements`, `Species`, `Phases` or `Constituent` must be used to indicate what is rejected.
`NAME&`	Names of the pre-defined elements, species, phases, and constituents
`ELEMENTS`	The given elements are restored.
`SPECIES`	The given species are restored and thus possible to form from the defined elements.
`PHASES`	The given phases are restored and thus possible to form from the defined elements or species.
`CONSTITUENT`	The given constituent in one phase are restored. Add the following when prompted: `Phase`: The name of the phase containing the constituent to be restored. `Sublattice number`: The sublattice where the constituent enters (the first sublattice is 1). `Constituent`: The name(s) of the constituent(s) to be restored.

SET_AUTO_APPEND_DATABASE

Enforce an automatic action that appends thermodynamic data from a chosen database regarding the system to the data you already have about the system from the current database (that is, the default database or the database last chosen with *SWITCH_DATABASE* on the next page or *APPEND_DATABASE* on page 12). This is useful to simultaneously retrieve both thermodynamic and mobility data for a defined system when performing a DICTRA module simulation.

This command should be used before defining a system (with the commands *DEFINE_ELEMENTS* on page 14, *DEFINE_SPECIES* on page 14, or *DEFINE_SYSTEM* on page 15) and retrieving the data with the *GET_DATA* on page 15 command from the primary switched database.

Syntax	SET_AUTO_APPEND_DATABASE
Prompt	`DATABASE NAME /XYZ/: <ADDITIONAL DATABASE NAME>`
Option	`ADDITIONAL DATABASE NAME` The name of an existing database or a USER database that corresponds to the automatically-appending database.

It works in a way that is similar to the APPEND_DATABASE<DATABASE-NAME> command sequence, but only the phases that are also available in the primary switched database are appended. There is no possibility to manually list, reject and/or restore any phase that is available in the appending database. When retrieving data with the GET_DATA command afterwards, all the phases that exist in the appending database but not in the primary switched database are automatically rejected. The prompt is kept as for the primary switched database, `TDB_XYZ`: (where `XYZ` stands for the name of the primary switched database) until the execution of the GET_DATA command.

Therefore, to selectively append more phases from a secondary database to a system that is defined and retrieved from a primary switched database, then the APPEND_DATABASE command and sequential commands (such as DATABASE_INFORMATION, DEFINE_SYSTEM, DEFINE_ELEMENT, DEFINE_SPECIES, LIST_SYSTEM, REJECT, RESTORE and GET_DATA) should be used instead, before this command.

Although it is impossible to manually list, reject and restore any phase from the appending database, the DATA module automatically ignores all the phases that do not exist in both the primary switched database and the appending database, and append the data for the phases (that are also available in the primary switched database) from the appending database, as informed on screen when executing *GET_DATA* on page 15 afterwards.

SWITCH_DATABASE

Switch (or change) from the current database to a new one, and reinitialize the entire DATA module for defining a system and the GES5 workspace for storing retrieved data. All the directly connected databases as predefined by the original database initiation file, or by a user-specified database initiation file after using *NEW_DIRECTORY_FILE* on page 17, are listed by pressing the <Enter> key without giving any argument. You can also supply your own database by giving the argument USER and then the database name and its correct path if it is not located in the current working directory. The second part of the prompt TDB_XYZ indicates the present database XYZ.

Syntax	SWITCH_DATABASE
Prompt	`DATABASE NAME /XYZ/: <NEW DATABASE NAME>` Use one of these databases: • `PURE` (SGTE pure element database) • `SSUB` (SGTE substance database 1997) • `USER` (user-defined database)
Options	**Description and Information**
`NEW DATABASE NAME`	The name of an existing database or a USER database definition file (***setup.TDB).
`DATABASE NAME`	The new database is specified by typing the abbreviation given in the front of one of the available predefined databases. When switching/appending databases or additionally purchased databases you can add these to the predefined database list in the database initiation file TC_INITD.TDB or initd.tdb of your installed software. When this command is used in a macro (*.TCM) file, if the USER option is selected, the database setup file name (*setup.TDB) that contains the setup definitions of the USER database, and its correct path, must be provided.
`FILENAME`	In Linux, the filename of a USER database, or one of the predefined names, can be used under this prompt. A valid filename for the USER database definition file (***setup.tdb) or a predefined database name, with the correct path. The default filename extension is .tdb.
Notes	If a USER database name or its path is not given on the same line of the SWITCH_DATABASE command, or if it is incomplete or incorrect, an Open window is displayed for the to-be-switched database. The USER database is used without reinitiating the Gibbs energy system, data from different databases can thus be combined. Therefore, the SWITCH_DATABASE USER command sequence is equivalent to the APPEND_DATABASE USER command sequence. The result of a combination must be examined carefully, because differences in standard states, phase models and names can be disastrous. If the same parameters occur in several such switched or appended databases, the last one retrieved is used in the calculations. It is not advisable to use this method for large databases since these load slowly. After this command, those commands for defining system (in terms of either elements or species), rejecting/restoring phases or species, retrieving data, as well as for appending data from additional database(s), can be proceeded.

EDIT_EXPERIMENTS Commands

These commands are accessed through the PARROT module.

Some special commands are designed only for the ED_EXP module and can also be used in *.POP or *.DOP files.

In this section:

Running the EDIT_EXPERIMENTS Command

To run the EDIT_EXPERIMENTS (ED_EXP) module:

- The first necessary command after entering the ED_EXP module for the first time (with *EDIT_EXPERIMENTS* on page 95 in the PARROT module) should always be READ_BLOCK in order to load the experimental data block from the current work *PAR-file for editing. Also, the read command must also be used prior to any other ED_EXP command if the module is reinitiated, or if no experimental data block has not previously been read from a work file compiled with a proper experimental data .POP/.DOP file, or if you want to change to another data block for editing.
- If any change is made in the ED_EXP module remember to use the command *SAVE_WORKSPACE* on page 232 before going BACK to the PARROT module.

Although the TABLE_HEAD, COMMENT and FLUSH_BUFFER commands are visible in the ED_EXP module, these cannot be used in the ED_EXP module; these are only functional in an *.POP or *.DOP file.

COMPUTE_ALL_EQUILIBRIA

In ED_EXP and PARROT modules, each experiment is treated as an individual equilibrium with some measured values. These are created with *CREATE_NEW_EQUILIBRIUM* on page 143, and stored in an experimental data *.POP file and then compiled and saved in the POLY3 workspace of a PARROT work *.PAR file.

With COMPUTE-ALL-EQUILIBRIA, all equilibria from the current to the last experimental points are calculated. If an equilibrium calculation fails, the calculation is stopped at that equilibrium. Equilibria with weight zero is skipped.

A current or present experimental point means the latest selected or calculated one. Once used the current point turns to the last point in the data block; in such a case you first use *SELECT_EQUILIBRIUM* on page 162 so that the current point is switched to a desired one.

Syntax	COMPUTE_ALL_EQUILIBRIA
	For this command there is always a list output on screen, which consists of six columns for all experimental points available in the current data block. The first column is the *equilibrium identifier* (a number) assigned by this command, the second the *data label* assigned with *LABEL_DATA* on page 28, the third the *number of iterations*, the fourth the *current weight*, and the fifth the *current temperature*. In the sixth column the *fixed stable phases* are listed together with any *comment text* given after a *COMMENT* on page 40 in the *.POP or *.DOP file. If the weight is zero for an equilibrium columns 3-5 are replaced by the text <*unused*>. If the alternate mode is used for some experimental points, the listing is slightly different for such points. The 3-4 columns are displayed with *alt*, instead. If an alternate calculation is failed at one experimental point, the point is automatically assigned with a zero weight, and a warning message is shown above the data line (with all six columns).

EXPERIMENT

This command is used in original experimental data files (*.POP or *.DOP), but can also be given interactively inside the ED-EXP module, to change the value or uncertainty of an experiment or to add more experimental information.

An experiment usually consists of two parts with a colon (:) separating them:

- as a quantity relation, and
- as the uncertainty of the value for the quantity,

The quantity relation can be a normal POLY-module condition or an inequality (which is similar to condition but the relation between the quantity and given value is not in equality, i.e. < or >). The uncertainty can be expressed as an absolute value or relative to the value (x%).

An experiment that uses an inequality gives zero contribution to the sum of errors in the optimization procedure of PARROT if the value is on the right side. If the value is on the wrong side, the value after the colon determines how steeply the error increases with the value.

Syntax	EXPERIMENT
	The experiment must be typed after the command. Several experiments can be given on the same line. The syntax of EXPERIMENT is similar to a CONDITION. Usually, a state variable set equal to a value with a given uncertainty is specified after the colon (:). For example, `T=1273.15:5`. An inequality, < or >, can also be used. For example: `ACR(C)<-0.01:0.001, W(BCC,AG)>0.05:10%`

Additional Information About the EXPERIMENT Command

A typical experiment added interactively specifies that a phase should not be stable in a certain experiment, because a phase may appear in a range of composition or of temperature where it has never been observed during the optimization. A phase is unstable if its driving force is negative, and you can add experimental information to enforce that. For example, you can suppress the HCP phase in an existing experimental point:

```
CHANGE-STATUS HCP=DORMANT
EXPERIMENT DGM(HCP)<-.001:.0001
```

`DGM` is the POLY variable for the driving force that is already divided by `RT`, and it is dimensionless. Only dormant phases can have driving forces larger than zero, as this indicates that these would be stable if allowed to form. The experiment in the above case tries to modify the model parameters to make the HCP phase unstable.

More general examples of experiment definitions:

```
EXPERIMENT X(LIQ,PB)=.10:.01 X(FCC,PB)=0.02:.01
EXPERIMENT ACR(PB)=0.8:5%
EXPERIMENT T=700:5
```

The first experiment above describes a tie-line where the experimentally measured mole fraction of Pb is 0.1 in the liquid phase and 0.02 in the FCC phase, and its uncertainty is 0.01 for both measurements. The second experiment is that the activity of Pb should be 0.8 with an uncertainty of 5 percent.

The reference state of the component Pb must be set with the command *SET_REFERENCE_STATE* on page 169. The final one is that the temperature should be 700 K with an uncertainty of 5 degrees.

Experiments that are functions of states variable(s) must be described as the defined functions. For example:

```
ENTER_FUNCTION HTR=HM(LIQUID)-HM(FCC);
EXPERIMENT HTR=7000:1000
```

EXPORT

Transfer/export a calculated value from an equilibrium to an optimizing variable in the PARROT workspace. Thus the value can be used, for example, in the Gibbs energy description of a phase. Of course, this variable should not be optimized (i.e. it should be set as a fixed variable in PARROT).

Syntax	EXPORT
Prompt	`FUNCTION NAME: <FUNCTION NAME>#<N>` Specify the name of the function, the value of which should be transferred to a `V` variable. The number (n) of the `V` variable must be given after the function name, separated by hash character #. The function name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.

	Example
	`ENTER_FUNCTION STRNGY=GM(FCC).X(CU);`
	`EXPORT STRNGY#6`
	This transfers the value of the partial derivative of the Gibbs energy of the FCC phase with respect to the mole fraction of Cu to the optimizing variable 6 (i.e. `V6`).

IMPORT

Transfer/import the value of one of the optimizing variables to a constant. Normally, it is directly used inside an experimental data (*.POP or *.DOP) file. It is the inverse of *EXPORT* on the previous page.

This is useful if several experiments are done at the same activity of a component, but this activity is not known. The activity should then be optimized and all equilibria with the same activity should use the same value. In this case the variable must be set as an optimizing variable, and an initial guess of the activity should be given. During the optimization, the PARROT program tries to find the activity that gives the best fit.

If an approximate value of the activity is known, it can be supplied as an experiment.

See example 36 in the *Console Mode Examples Guide*.

Syntax	IMPORT
Prompt	`CONSTANT NAME: <CONSTANT NAME>#<N>` The value of the `V` variable must be assigned a symbolic constant. The number (`n`) of the `V` variable must be given after the constant name, separated by hash character `#`. The constant name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.

	Example
	`ENTER_CONSTANT ACU=0.1`
	`IMPORT ACU#2`
	This transfers the value of the optimizing variable 2 (i.e. `V2`) to the constant `ACU`.

LABEL_DATA

Add a label to the experimental equilibrium point, either as a single point or several points given individually or in a table. The label is maximum four characters and must start with the letter A. Normally, it is directly used inside an experimental data (*.POP or *.DOP) file.

Several experimental equilibria can be given the same label, and the label can be used in the command *SET_WEIGHT* on page 33 to assign the same weight to all equilibria with the same label.

Syntax	LABEL_DATA
Prompt	`LABEL? /A1/: A<BCD>` Specify a textual label (as maximum characters and must start with the letter `A`) for the current experimental equilibrium point(s).

LIST_ALL_EQUILIBRIA

Syntax	LIST_ALL_EQUILIBRIA
	List all the details (including equilibrium indicators, labels, iteration numbers, weight, and fixed phases or comments) of all equilibrium points from the current one to the last one on screen. You can always use *SELECT_EQUILIBRIUM* on page 162 to select a specific point as the current equilibrium point for such a list.

MAKE_POP_FILE

It is possible in the ED_EXP module to make interactive changes and additions to the original experimental data file (the *.POP or *.DOP file).

To document or transfer the current or final experimental data to a *.POP/*.DOP file, you can use this command to write it to a new *.POP/*.DOP file or overwrite it on an old one.

Check this output carefully for errors. Tables in original *.POP/*.DOP files are written as individual experimental points. The output can be shown on screen or be saved as a new *.POP file where to write or overwrite the edited experimental information in a simple text format.

If an existing *.POP file name is specified, it is overwritten. In the DICTRA module, an *.DOP file is written or overwritten.

Syntax	MAKE_POP_FILE
Prompt	`OUTPUT TO SCREEN OR FILE /SCREEN/: <POP/DOP-FILE NAME>` Specify a name of the new *.POP/*.DOP file where to write or overwrite the edited experimental information in a simple text format.

READ

This command must be given each time the ED_EXP module is entered, unless it is already given once in ED_EXP and does not use *LIST_RESULT* on page 104 or *OPTIMIZE_VARIABLES* on page 109 in PARROT in between.

Syntax	READ
Prompt	`BLOCK NUMBER /#/: <N>` The number of data block that should be edited must be given. If there is no command *FLUSH_BUFFER* on page 41 in the original POP or DOP file, then there is only one data block with the number 1.
	READ_WORKSPACE = READ This command (previously named READ_BLOCK) is equivalent to *READ_WORKSPACE* on page 232 in the POLY module, but it only reads the POLY3 workspace from the work file set by *SET_STORE_FILE* on page 116 in the PARROT module.

RESTORE_ALL_WEIGHTS

Restore a specific weight-set (previously saved by *STORE_ALL_WEIGHTS* on page 34) and assign all the different experimental points in the current data block with the previously-set weights in the sequential assessments.

Syntax	RESTORE_ALL_WEIGHTS
Prompt	`SET NUMBER (0 FOR LIST) /0/: <WEIGHT-SET NUMBER>` The default value 0 is for a list on screen.

SAVE_WORKSPACES

In the PARROT workspace this command saves the current status of the EDIT_EXPERIMENT submodule before you switch back to the PARROT module. This is required when you want to save equilibria changes, including changes to conditions, experimental data, and/or computed equilibria results, as well as any newly added equilibria.

With this command all the changes made in the EDIT_EXPERIMENT submodule are saved in the PARROT workspace. This means you do not need to execute *SAVE_PARROT_WORKSPACES* on page 111 in the PARROT module.

However, when in the PARROT module, additional changes can only be saved with the SAVE_PARROT_WORKSPACES command even if they have been made prior to executing SAVE_WORKSPACES in the EDIT_EXPERIMENT module.

When you exit the EDIT_EXPERIMENT module (or Thermo-Calc), the next time the file is opened it is in the same state as when you executed the SAVE_WORKSPACES command. However, if you use *OPTIMIZE_VARIABLES* on page 109 the computed results are automatically updated.

Syntax	SAVE_WORKSPACES
Prompt	`<FILE NAME> <Y OR N>` Sometimes good starting values (*SET_START_VALUE* on page 171) are required to successfully get or compute an equilibrium correctly. In this case, it is important to save the computed equilibrium in the PARROT workspace. It is important to remember that the computed results can be ruined by improper optimizations. For this reason, it is suggested you save the PAR file with a different name to back up the PARROT workspace.

SET_ALTERNATE_CONDITION

A special command used in the experimental data *.POP/*.DOP file but also possible in the ED_EXP module. It is used only when you have specified that the alternate mode is set in the PARROT module.

The command syntax is almost the same as for the POLY command *SET_CONDITION* on page 165 while the uncertainty should also be specified.

The alternate condition (including the normally POLY-module condition plus uncertainly; see below) must be given explicitly, but can be given on the same line or on separate lines with each one started with the command.

Syntax	SET_ALTERNATE_CONDITION
Prompt	`STATE VARIABLE EXPRESSION: <STATE VARIABLE NAME OR LINEAR EXPRESSION>` Give either a state variable or a linear expression of state variables.
Options	**Description and Information**
State variables	Some of the state variables that can be used in conditions are: • `T` (temperature in the system) • `P` (pressure in the system) • `N` (system size in moles) • `B` (system site in grams) • `W(<component>)` (mole fraction of a component in the system) • `X(<component>)` (fraction of a component in the system) • `ACR(<component>)` (activity of a component in the system) • `MUR(<component>)` (chemical potential of a component in the system) • `W(<phase>,<component>)` (mole fraction of a component in a phase) • `X(<phase>,<component>)` (mass fraction of a component in a phase) • `ACR(<phase>,<component>)` (activity of a component in a phase) • `MUR(<phase>,<component>)` (chemical potential of a component in a phase) • `H` (enthalpy in the system) • `HM(<phase>)` (enthalpy of a phase per mole)

Additional prompts	`FACTOR: <A FACTOR FOR THE STATE VARIABLE, OR A CONTINUATION>`
	This question means that the previous question was not answered. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:
	`2*MUR(FE)+3*MUR(O)=-35000`
	This means that it should be a condition that two times the chemical potential of FE plus

Syntax	SET_ALTERNATE_CONDITION
	three times the chemical potential of O should be -35000 J/mol.
	`STATE VARIABLE: <A SPECIFIED STATE VARIABLE, OR A CONTINUATION>` This question is prompted if a single state variable name has not given in either the prompt `State variable expression` or `Factor`, or a state variable expression is given but the expression is incomplete, for example, `T-` or `2*MUR(FE)+`, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).
	`VALUE /X/:  <A NUMERIC VALUE, A CONSTANT OR A VARIABLE>` The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value `NONE` means that the condition is removed.
	`UNCERTAINTY /NONE/:  <UNCERTAINTY OF THE CONDITION>` The uncertainty of the condition. This can be a numeric value, a constant or a variable. The default value `NONE` means that the uncertainty for the value specified above is zero. The uncertainty can either be expressed as an absolute value or relative to the value of the condition in percent (`x%`).

Notes	There are more state variables that can be used in conditions. For more information, type an INFO STATE_VARIABLES command in the POLY module. A condition is normally a value of a single state variable with its value.
	For example:
	`T=1273.15  P=1E5`
	`X(C)=.002`
	`W(CR)=1.5`
	`ACR(CR)=0.85`
	`X(FCC,C)=.001`
	`H=-250000`
	`HM(BCC)=-225000`
	A condition can also be a value of a linear expression involving more than one state variable.
	For example:
	`X(LIQ,S)-X(PYRR,S)=0`

Syntax	SET_ALTERNATE_CONDITION
	This means that it is a condition that the mole fraction of `S` should be the same in the LIQUID and PYRRHOTITE phases. In practice that should be the congruent melting point. After the equal sign only a numeric value is allowed.

SET_WEIGHT

Each experimental value has an uncertainty associated with it, specified by the value after the colon (:) with the command *EXPERIMENT* on page 24. During an optimization the absolute difference between the experimental and calculated values gives a contribution to the sum of error.

With the SET_WEIGHT command, you can change the scale of such a contribution (the uncertainty) for a single experimental point, or the contributions (all uncertainties) for a set of equilibria. The default weight is always unity. A value smaller than one means that the experiments should have less weight. A value larger than one that these should have higher weight. The special value zero means that the set of equilibria should be ignored in editing in ED_EXP (as *COMPUTE_ALL_EQUILIBRIA* on page 23 is given) and in *OPTIMIZE_VARIABLES* on page 109 in PARROT.

The weight may be needed to obtain a balance between different kinds of experiments. For example, if there are only five experimental values of the composition of a phase diagram but 500 experimental values of activities or enthalpies, then the five composition points may have to be given higher weight than unity, otherwise these are not well described by the optimizing procedure.

Syntax	SET_WEIGHT
Prompts	`VALUE /1/: <WEIGHT VALUE>` Specify a weight of the experiments in the specified equilibria (asked in the next prompt). The contribution to the sum of errors of these experiments are multiplied by this weight. The weight is squared, thus use 0.7 to make the error half (0.49) as big, and 1.4 to make it twice (1.96) as large.
	`EQUILIBRIA (RANGE) OR LABEL(S) /PRESENT/:<SELECTION>` Define the equilibria. These are available in the read data block from the current work file and are given the above-defined weight. The selection may be given as a range but the equilibrium numbers must then be separated only by a minus sign.

Syntax	SET_WEIGHT
	The start and end equilibrium numbers must be available in the read data block read from the current work file. For example, `5-101`, means that all equilibria starting from the identifier 5 until the identifier `101`. Some of numbers between these two identifiers may not exist in the data block. The selection may also be given as one or more labels (which should be separated only by a space). All equilibria with the specified label(s) in the read data block are given the above-defined weight. By pressing <Enter> to accept the default value `present`, the above defined weight is only assigned to the current or present experimental point (which is selected by the POLY command *SELECT_EQUILIBRIUM* on page 162). If *COMPUTE_ALL_EQUILIBRIA* on page 23 is used but no specific equilibrium point is selected afterwards, the last point in the read data block remains the `present` point.

STORE_ALL_WEIGHTS

Store a new weight-set that is the current situation of specified weights for all the different experimental points read from the currently-selected experimental data block in an assessment. This is useful when you want to try various weight-settings for some experimental points or for all the points, and then compare the assessment results from different weight-sets. Such a saved weight-set can be recalled and restored for all experimental data point with*RESTORE_ALL_WEIGHTS* on page 29 sequentially.

Syntax	STORE_ALL_WEIGHTS
Prompt	`COMMAND LINE: <WEIGHT-SET NAME>` Give a weight-set name (comment line texts) for the current weight set for all experimental points.

TRANSFER_START_VALUE

In the ED_EXP module it is time consuming to calculate all equilibria when the optimization is sensitive to start values of the composition of the phases. Usually in one data block there are several experimental points with the same kind of equilibrium and each must have its start value set. When you manage to calculate equilibriums of such experimental points, this command is useful to transfer the site fractions from a successfully-calculated equilibria to the present experimental point.

Syntax	TRANSFER_START_VALUE
Prompt	`FROM EQUILIBRIUM /PREVIOUS/: <EQUILIBRIUM NUMBER>` The equilibrium number is the numeric identifier for the equilibrium from which the start values should be copied to the present experimental point. `Previous` is the default if you press <Enter>.

Experimental Data Files

In this section:

Commands in the Experimental Data Files (*.POP, *.DOP)

In order to conduct an assessment for a system, the experimental data is described with a syntax, which is similar to the way that one calculates an equilibrium in the POLY module or you edit an experimental point in the ED_EXP module. Similar to a Thermo-Calc (TCC) macro file (*.TCM), an experimental data file (i.e. the *.POP or *.DOP file) is a basic text file and can be opened and edited by any text editor. For this reason, an *.POP or *.DOP file is not hardware dependent.

A POP or DOP file consists of various commands from the POLY and ED_EXP modules, as well some special commands which can only be used in such experimental data files. Various experimental information can be inputted in an *.POP or *.DOP file as different tables; the same type of experimental data are usually documented in the same table (see below).

An *.POP or *.DOP file is used in the PARROT module to provide experimental information for the optimization process, and is checked by a *syntax checker* when the PARROT command *COMPILE_EXPERIMENTS* on page 92 is proceeded.

Many POLY and ED_EXP commands can be directly used in a POP or DOP file. But there are some differences with the set of POLY or ED_EXP commands, and some specially designed commands as described in this topic can only be used in the *.POP or *.DOP files.

Frequently Used Commands

Most of the commands in the experimental data file are the same as in the POLY module. The most frequently used are listed below:

- *CREATE_NEW_EQUILIBRIUM* on page 143
- *CHANGE_STATUS* on page 135
- *SET_CONDITION* on page 165
- *SET_REFERENCE_STATE* on page 169
- *ENTER_SYMBOL* on page 195
- *SAVE_WORKSPACES* on page 30

As the last command in an *.POP or *.DOP file, you must always have the SAVE command.

Other Commands

Other legal commands from the POLY module that are used less often are:

- *DEFINE_COMPONENTS* on page 143
- *EVALUATE_FUNCTIONS* on page 155

- *SET_ALL_START_VALUES* on page 162
- *SET_NUMERICAL_LIMITS* on page 237
- *SET_START_VALUE* on page 171
- *ADVANCED_OPTIONS* on page 125

The DEFINE-COMPONENTS command must be always used as the first command in an *.POP or *.DOP file, as it automatically reinitiates the whole workspace.

Most of the special commands for the ED_EXP module are also often used in an *.POP or *.DOP file. For example:

- *EXPERIMENT* on page 24
- *EXPORT* on page 26
- *IMPORT* on page 27
- *LABEL_DATA* on page 28
- *SET_ALTERNATE_CONDITION* on page 30
- *SET_WEIGHT* on page 33

The following special ED_EXP commands are illegal and should not be used in any *.POP or *.DOP file:

- COMPUTE-ALL-EQUILIBRIA
- MAKE-POP-FILE
- READ (READ-BLOCK OR READ-WORKSPACE)
- TRANSFER-START-VALUES

The special commenting identifier, i.e. a single dollar sign $ which starts a line, is used to document comment lines at any position in an *.POP or *.DOP file. You may remember that this feature is universally the same as in almost all kinds of text files in Thermo-Calc software, e.g. in *.TDB, *.DAT, *.TCM, *.POP/*.DOP and *.EXP files. Such a sign and all information afterwards in the same comment line is skipped and ignored by the syntax checker. Therefore, you shall feel free to write such comment lines in any of these types of text files.

TABLE_HEAD, TABLE_VALUES and TABLE_END

These commands are used only in the *.POP/*.DOP files. It represents a convenient way to enter many experimental measurements of the same type in a table format.

> These commands should always be used together and in a sequence, meaning that a table should always start with the TABLE-HEAD command, then follows the TABLE-VALUES command, and finish by the TABLE-END command. Between the two TABLEHEAD and TABLE-VALUES commands, there should exist some definition lines (e.g. on phase status, reference states, conditions, experiments, labels, etc.) for the experimental measurements of the current information type.

Syntax	TABLE_HEAD TABLE_VALUES TABLE_END
Prompt	

After the TABLE-HEAD command, there must be an equilibrium description similar to a single experimental equilibrium but with some special notation. Then, there is always a TABLE-VALUES command, after which the actual data is given in columns. At the end of each table, there must be a TABLE-END command.

The TABLE-HEAD command must be followed by a numeric value. This is used to generate unique numeric identifiers for all the equilibria in the table. The numeric identifier is incremented by one for each experimental (equilibrium) point in the table.

Example

An example of the use of a table for enthalpy measurements in the liquid is given here. Much more elaborate tables can be used

```
$ Enthalpies of mixing, Topor and Kleppa, Met Trans 1984 TABLE-HEAD 1
CREATE—NEW @@ 1
CHANGE-STATUS PHASE LIQ=FIX 1
SET-REFERENCE-STATE AU LIQ * 1E5
SET-REFERENCE-STATE CU LIQ * 1E5
SET-CONDITION P=1E5 T=1379 X(LIQ,AU)=@1
LABEL ALH
EXPER HMR=@2:5%
TABLE—VALUES
```

Syntax	TABLE_HEAD TABLE_VALUES TABLE_END

```
0.0115 -322
0.0563 -1520
0.8499 -2976
0.9002 -2114
TABLE—END
```

The equilibrium description between TABLE-HEAD and TABLE-VALUES is similar as for a single experiment, except for these details:

- @@ Used to automatically generate a series of identifying numbers instead of creating only one with the command *CREATE_NEW_EQUILIBRIUM* on page 143. The program automatically generates the identifying numbers starting after the number given after the TABLE-HEAD command (in this case it is 1).
- @1 values in the table are specified by an @ sign followed by a column number. In the above case, the mole fraction of Au in the liquid is in column 1 (see the line for SET-CONDITION). The columns may have other information than values, and you can use phase names or any text. If the text contains spaces or special characters, it must be surrounded by double quotes in the table, e.g. “`ABC DEF&ghi`”.
- For the *syntax checker* all commands describing the equilibrium must be in UPPER case after the TABLE-HEAD command.
- After the TABLE-VALUES command, there should be one line for each experimental measurement of the same type giving the values or texts that should be copied into the places of the condition or experiment defined by `@1`, `t`, etc. You can have columns that are not used but there must be exactly the same number of columns of each line, otherwise the syntax checker gives an error message in the PARROT module.

COMMENT

This command is only used in the *.POP/*.DOP files to write brief comments or descriptive information on a newly created equilibrium (experimental) data point or a set of points given in a table.

Syntax	COMMENT
	A comment can have a maximum of about 60 characters written on the same line.

FLUSH_BUFFER

This command is only used in the *.POP/*.DOP files. It is needed if the number of experiments require more space than can be fitted into one buffer. When the PARROT program compiles experiments, it informs if any FLUSH commands are needed. The FLUSH_BUFFER command terminates the current block, save it to the work file and starts a new block. With the READ command in the EDIT-EXP module, you can select the block to edit.

Syntax	FLUSH_BUFFER
	After a FLUSH_BUFFER command, the workspace is reinitiated and all functions or constants must be entered again in the *.POP file. You can take advantage of this; for example, you can use the FLUSH command to have blocks with different components in one *.POP file.

GIBBS_ENERGY_SYSTEM Commands

In this section:

ADD_COMMENT

Syntax	ADD_COMMENT
	Add a comment or make notes about parameters.

AMEND_ELEMENT_DATA

The data for an element (in the SER, the Stable Element Reference, state) can be changed by this command. It should only be used for the elements that do not have any data in the database because the element data available in the database is set by the database-developer for the purpose of internal consistency. Except for the mass, the other values have no influence on the calculations.

Syntax	AMEND_ELEMENT_DATA
Prompts	`ELEMENT NAME: <ELEMENT NAME>` Specify the name of the element for which you want to change the data.
	`NEW STABLE ELEMENT REFERENCE /ABCD/: <NAME OF SER>` Press <Enter> to accept the default `SER` or specify a new SER for the element. Important: The default name should not be changed if this data is retrieved from a database. This name is used when parameters for a phase are listed and the database assumes that the stable element reference is the same as in the database. Only if the element's data have not been fetched from a database, e.g. entered manually, can you enter a new SER.
	`NEW ATOMIC MASS /XX.XXXX/: <YYYYYY>` Press <Enter> to accept the default atomic mass or specify a new value for the element. The atomic mass of the element is given in g/mol.
	`NEW H(298.15)-H(0) /XXX.XXX/: <YYYYY>` Press <Enter> to accept the default H(298.15)-H(0) or specify a new value for the element. H(298.15)-H(0) is the enthalpy difference between 298.15 K and 0 K for the element in its SER state.
	`NEW S(298.15) /XX.XXXX/: <YYYYY>` Press <Enter> to accept the default S(298.15) or specify a new value for the element. S (298.15) is the absolute value of the entropy at 298.15 K for the element in its SER state.
	`DEFAULT ELEMENT REFERENCE STATE SYMBOL INDEX /#/: <INDEX>` The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data, you must set the index to get the correct symbol.

Syntax	AMEND_ELEMENT_DATA
	Specify an index for the default listing parameters (symbol), or press <Enter> to accept the pre-set index. 0 is for `G`, 1 is for `H298` and 2 is for `H0`. The index is to define the symbol printed in parameter listings. The symbol can be: • `G` the data are referred to Gibbs energy at a variable temperature (also called *lattice stability*). • `H298` the data are referred to the enthalpy of the element at 298.15 K and 1 bar. • `H0` is the same as `H298` but at the temperature 0 K.

AMEND_PARAMETER

Use this command to interactively change/amend the temperature-pressure function of a parameter. This is useful to correct typing errors because the old function is made available on the terminal for interactive editing. For most of these prompts, refer to *ENTER_PARAMETER* on page 99 for details.

This AMEND_PARAMETER command is for the GES module. There is also a PARROT module command with the same name (*AMEND_PARAMETER* on page 88).

Syntax	AMEND_PARAMETER

Prompts	`PARAMETER: <PARAMETER NAME>`
	Specify a correct parameter name. If a parameter name is not acceptable or you only press <Enter>, the error message displays:
	`ERROR, PLEASE RE-ENTER EACH PART SEPARATELY`
	The program prompts for separate input for each part for a parameter name.

	`IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK>` Specify one of these legal identifiers as described for ENTER_PARAMETER.
	`PHASE NAME (/ABCD/): <PHASE NAME>` Specify the phase name.
	`CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME>` Specify the constituent name.
	`INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME>` Specify the interacting constituent name: If there is no interacting constituent, press <Enter>.

Syntax	AMEND_PARAMETER
	`INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME>` If there are more than one interacting constituents, specify them; otherwise press <Enter>.
	`DEGREE /#/: <DEGREE>` Specify a numerical number as the degree of the phase parameter.
	After the parameter name is specified correctly, the program lists its current definition (either present in the database or defined by the ENTER_PARAMETER command), such as:

```
L(PHASE2,AL,MG;1)=

298.15<T<2000.00: +5000

2000.00<T<4500.00: +4500

4500.00<T<6000.00: +4000
```

Then you are prompted to change the parameter definition, as shown below:

```
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: <Y OR N>
```

If you want to change the number of ranges for the chosen function, or change some of the temperature limits in the definition, for Y, retype both the low/high temperature limits and functions.

If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press <Enter> to accept the default N, then the whole definition of the chosen parameter in all ranges (if any) is listed on screen, such as:

```
DIFFERENT FUNCTIONS IN THESE RANGES

298.15<T<2000.00

2000.00<T<4500.00

4500.00<T<6000.00
```

The prompt is given:

```
DO YOU WANT TO CHANGE RANGE LIMITS /NO/: <Y OR N>
```

If there is more than one range, this question is prompted press <Enter>.

	`RANGE NUMBER (0 TO EXIT) /0/: <RANGE NUMBER>` If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any changes.
	`FUNCTION:`

Syntax	AMEND_PARAMETER

The previous function is available for editing. The editing is performed within the general subroutine FOOLED, as described in *AMEND_SYMBOL* on page 90. This routine prompts as follows:

```
1:+:>
```

The prompt consists of the current position in the string and the character at that position between colons, (::).

Commands

These commands can be given:

- Help: `?`
- Move CP to last or first character: `<+/-> A`
- Delete characters from CP: `<+-#characters> D`
- Exit: `E`
- Find: `<#occurrences> F<string>@`
- Insert: `I<string>@`
- Move: `<+-#positions> M`
- Restore string: `R`
- Substitute: `S<OLD>@<NEW>@`
- Type string: `T`

Where CP denotes the current position in string, # means number of, @ is a terminator of an input or search string.

When the string is typed the character at the current position is replaced by an underscore _.

To finish the editing of the current function, type `E` at the prompt.

Solution Models in the GIBBS Module

The command *AMEND_PHASE_DESCRIPTION* on page 52 is used to specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

This topic outlines the application of each option and includes important information about each command.

There are many solution models implemented in the GIBBS module (type `INFO MODELS` to see details about various thermodynamic models). However, these are switched on and handled differently via various GIBBS routines/commands:

- The first models the non-ideality as excess parts, i.e. by amending the phase’s EXCESS_MODEL and/or TERNARY_EXTRAPOLAT models.
- The second models the non-ideality as ADDITIONAL parts, i.e. by amending the phase’s other subjects in this command, e.g. MAGNETIC_ORDERING for the Magnetic Ordering Model, DISORDERED_PART for the CVM Approach in modelling chemical ordering/disordering phenomenon, QUASICHEM_IONIC for using a quasi-chemical entropy term for an ionic two-sublattice liquid solution phase, QUASICHEM_FACT00 or QUASICHEM_IRSID for describing a substitutional liquid solution phase, DEBYE_HUCKEL for the DHLL/SIT Model in describing a dilute aqueous solution phase, etc.
- The third implements the model entirely or partially into the GIBBS module and related database(s), such as for the electrostatic contribution in an AQUEOUS solution phase by the Complete Revised_HKF Model, the Murngham Model, Birch-Murngham Model or Generalized PVT Model for high-pressure/temperature volume contribution in a solid or liquid phase, the SUPERFLUID Model for the non-ideal EOS and non-ideal mixing in a gaseous mixture.

NEW_CONSTITUENT

Use this if you want to add a new constituent to a phase. It is illegal to add new constituents to an ionic two-sublattice liquid phase.

RENAME_PHASE

Use this to change the names of some specific phases. For example, a phase called *FE3O4_S* may be better named *Magnetite* to help identify it during the calculations and postprocessing. This is also a way to delete a phase by hiding it under a new name.

SITE_RATIOS

Use this to change the number of sites (i.e. the stoichiometric coefficients of various sublattices) in a sublattice phase.

COMPOSITION_SETS

Use this for solution phases that may have miscibility gap(s). However, this is less important today and often unnecessary to define additional composition set(s), since the implemented Global Minimization Technique can usually detect and add such composition set(s) in an automatic manner where it is really necessary during equilibrium calculations (of single-points, stepping or mapping).

MAJOR_CONSTITUENT

Use this to set major constituent(s) on each sublattice in each composition set for a solution phase. This is useful to make calculations converge faster because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set. The databases often set major constituents for several phases automatically when data are retrieved.

FRACTION_LIMITS

Use this to limit the application range (in terms of mole-fractions of all the involved elements) of a particular solution phase. This is useful to avoid automatic creations (enforced by the Global Minimization Technique) of additional composition sets for some solution phases (such as AQUEOUS solutions or dilute Fe-based liquid mixtures) of which the used models [e.g. the `SIT Model` or the `Complete Revised_HKF Model` for AQUEOUS solution, or the modified dilute solution parameters (plus a quadratic term, according to Hillert (1986) based on the SigworthElliot Model (Sigworth and Elliot, 1974) for Fe-rich liquid mixture] cannot be appropriately applied on a full scale.

Globally set the composition limits (in terms of mole fractions of various elements) in a specific solution phase, so that whenever the program finds a potential phase composition or a new composition set of possible miscibility gap(s) but that is out of this globally-set composition range, the program automatically ignores such a phase composition in an equilibrium calculation. This can be done either permanently inside a database (by enforcing this option for amending the phase-description of the solution phase) or temporarily within the GIBBS module (by using this phase-description amendment option).

This is important for solution phases for which the thermodynamic models and assessed data for the phases are for specific composition ranges, for example, the FE_LIQUID phase in the SLAG database is only applicable for Fe-rich liquid mixture, and the AQUEOUS phase in the TCAQ/PAQ and AQS/PAQS databases is only applicable for H2O-dominant aqueous solution phase.

Specify the low and high mole-fraction limits for each of the elements possibly available within the considered phase (in the currently defined system, or in a certain database). Do this for all the possible elements (defined in the phase) in a single AMEND_PHASE_DESCRIPTION FRACTION_LIMITS command-sequence, for example:

```
TYPE_DEFINITION R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS Fe 0 0.6
      Ag 0 0.01  Al 0 0.05  Ca 0 0.05  Co 0 0.01  Cr 0 0.01
      Cu 0 0.02  Mg 0 0.05  Mn 0 0.05  Mo 0 0.05  Nb 0 0.05
      Ni 0 0.05  Pb 0 0.05  Si 0 0.10  Sn 0 0.02  Ti 0 0.05
U  0 0.01  V  0 0.02  W  0 0.02  Zr 0 0.03
      B  0 0.01  C  0 0.01  H  0 0.01  N  0 0.01  O  0 0.01
P  0 0.01  S  0 0.01  !
```

DISORDERED_PART

This command is needed for the special treatment of chemically-ordered phases where the contributions from the disordered state are described by a phase without ordering sublattices (the disordered phase name must be specified).

Several checks are made that the ordered and disordered phases are compatible (sublattices, sites and constituents). A link is then created between the phases, and the disordered phase is hidden from application programs. The Gibbs energy for the ordered phase also includes the Gibbs energy for the disordered phase.

Phases which can have an order/disorder transformation have parameters split on two phases and are referred to as the *two phase* description in the GIBBS module. One of them has sublattices for chemical ordering, the other one represents the disordered state. Normally, the ordered BCC and FCC or HCP phases may have either 2 or 4 substitutional sublattice (plus one additional interstitial site), that are handled by the Two Substitutional-Sublattice Ordering Model or Four Substitutional-Sublattice Ordering Model, respectively.

Two phase means that the *ordered* phase has parameters that describe the ordering. The *disordered* phase has all parameters for the reference state and those for describing the disordered phase. The ordered phase may occur only is some systems whereas the disordered phase may occur frequently, typical examples are the disordered FCC and BCC which may become ordered as L12 or B2 in certain systems. In order to treat multicomponent systems where some subsystems have ordering it would be necessary to transform all parameters of BCC into a B2 model.

The parameters describing the disordered phase are not changed but the Gibbs Energy system is informed that the Gibbs Energy for the two phases should be added.

The method used calculates the Gibbs Energy of a two phase model with two or four substitutional sublattices for ordering.

$$G_m = G_m^{ord}(y_i^{'}, y_i^{''}) + G_m^{dis}(x_i) - G_m^{ord}(y_i^{'} = x_i, y_i^{''} = x_i)$$

The mole fractions *x*i are calculated from the site fractions *y*i. The last term means that the contribution from Gmord in a disordered state (same site fraction, equal to the mole fraction, on both sublattices) is subtracted. The effect of this is that the parameters in the ordered phase have no contribution to the disordered state.

MAGNETIC_ORDERING

Change the magnetic ordering parameter for a certain phase with magnetic ordering contribution, in terms of its anti-ferromagnetic factor. By default this is –1 for BCC phase and –3 for all other phases (FCC, HCP, etc.). The fraction value of the total enthalpy (due to short-range ordering above the magnetic transition temperature) is by default 0.40 for BCC phase and 0.28 for all other phases (FCC, HCP, etc.).

EXCESS_MODEL

Use this to change the default Excess Model (for interaction energies) from the default (REDLICH-KISTER_MUGGIANU). The model handles the excess interaction energies in a solution phase is chosen from:

- REDLICH-KISTER_MUGGIANU: for binary (R-K) & ternary (R-K-M) interactions
- REDLICH-KISTER_KOHLER: for binary (R-K) & ternary (R-K-K) interactions

- FLORY-HUGGINS POLYMER MODEL: for interactions in a polymer mixture phase (F-H)
- MIXED-EXCESS-MODELS: (R-K default) for mixed binary excess model (R-K, Legendre & Polynom) of a substitutional solution phase
- HKF: for interaction in an AQUEOUS solution phase (HKF)
- PITZER: for interaction in an AQUEOUS solution phase (PIT)
- CENTRAL_ATOM_MODEL: for interaction in a liquid slag solution phase (C-A-M)

For extrapolations of excess energies from related binary systems to ternary or higher-order systems, the Redlich-Kister binary excess interaction parameters may be extrapolated with either a Muggianu extension (i.e. the default REDLICH-KISTER_MUGGIANU model) and a Kohler extension (i.e. the alternative REDLICH-KISTER_KOHLER model), where there is no ternary, quaternary or higher-order interaction parameter.

The REDLICHKISTER_KOHLER model is implemented only for ternary systems.

The MIXED-EXCESS-MODELS option works only for a substitutional phase with no sublattice (such as the metallic LIQUID phase) and it can be used to invoke asymmetrical simple or Legendre polynomial as binary excess energy models in addition to the default symmetrical Redlich-Kister model for the chosen pair of constituents in a substitutional phase with no sublattice. Asymmetrical here means that the power series depend only on one of the constituents, for example with expansions based on the [1-2*X(B)] term rather than [X(A)X(B)].

Binary interaction parameters for such a pair of constituents must be entered prior to turning on the non-default Legendre or Polynom models.

See example 52 in the *Console Mode Examples Guide*for an example.

TERNARY_EXTRAPOLAT

Use this to change the extrapolation method from the default REDLICH-KISTER_MUGGIANU to another extrapolation model. This method extrapolates from binary to ternary (and higher-order) excess interaction parameters in a solution phase and is chosen from:

- MUGGIANU for Muggianu Extrapolation from R-K parameters
- TOOP-KOHLER for Toop-Kohler Extrapolation Model
- KOHLER-ALL for Kohler Extrapolation Model
- MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model

Only when all the relevant binary excess energies in the current solution phase are treated by the default Redlich-Kister Model (i.e. the Mixed-Excess-Model should have not been used), the MUGGIANU_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method to the RedlichKister_Kohler Model.

The default ternary extrapolation method MUGGIANU_RESTOR applies to a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister_Muggianu Model (in short as R-K-M), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such a default R-K-M Model is always used.

The KOHLER-ALL ternary extrapolation method can be turned on also for a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model.

REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister_Kohler Model (in short as R-K-K), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such an R-K-K Model is used.

The TOOP-KOHLER ternary extrapolation method is applied in a special way: for a specific ternary system (e.g. A-B-C) in a solution phase, specify which two constituents as the so-called Kohler constituents and the remaining constituent as the so-called Toop constituent on a given sublattice. If for the A-B-C ternary system you have specified A and B, or B and A, as the Kohler constituents (entered as the basis constituent and first interacting constituent) and C as the Toop constituent, only the A-B binary interaction parameters are used in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction parameters involving the Toop species C (i.e. of A-C and B-C binaries) are used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions).

This concept is shown in the *Console Mode Examples Guide*.

DEBYE_HUCKEL

To use the DHLL (Debye-Hückel Limiting Law) model and SIT (Specific Ionic Interaction Theory) model for a dilute AQUEOUS solution phase, switch the DEBYE_HUCKEL part on, and it removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS phase.

HKF_ELECTROSTATIC

To use the hypothetical electrostatic contribution for the chosen phase (it must be an aqueous solution phase using the Complete Revised_HKF Model). It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS solution phase.

QUASICHEM_IONIC

To use the Quasichemical-Ionic model for the chosen liquid phase, you must have already entered/retrieved a liquid phase as an ionic two-sublattice liquid solution phase (normally, that is the IONIC_LIQ phase), and then use this amending option to switch QUASICHEM_IONIC on. It creates a completely new liquid solution phase [namely the QUAS_IONIC phase which uses the Quasichemical Model for the entropy, according to Mats Hillert (2001: *J of Alloys and Compounds*, 320, 161-176)], while the original IONIC_LIQ phase remains in the system and is not changed by this option.

QUASICHEM_FACT00

To use the Quasichemical Model developed by Kongoli et al. in the F*A*C*T group in Montreal, you must have entered/retrieved a liquid phase using a normal substitutional liquid model with specified associates or species (on a single lattice site), and then turn on the option QUASICHEM_FACT00. This removes the previously-set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.

See examples 49 and 50 in the *Console Mode Examples Guide*.

QUASICHEM_IRSID

To use the Kapoor-Frohberg-Gaye Quasichemical Cell Model (i.e. the Quasichemical Model developed by ISRID, France) for a liquid SLAG solution phase, you can use a normal liquid model with specified associates or species.

GLASS_TRANSITION

To use the special model for glass transition of a liquid phase. It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.

REMOVE_ADDITION

To remove all the selected ADDITIONAL part from the Gibbs energy description for the chosen phase. If preferred, set a specific phase-status bit for a phase, use the PHASE_BITS option as long you know the restrict meaning of each part of a phase- status bits.

DEFAULT_STABLE

Set phases as default-stable, which helps you to have a better guess of which phases that should be stable at the first calculation.

AMEND_PHASE_DESCRIPTION

Specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

Also see *Solution Models in the GIBBS Module* on page 46 for detailed information about this command and its options.

Syntax	AMEND_PHASE_DESCRIPTION

Prompts	`PHASE NAME: <PHASE NAME>`
	Specify the name of the phase.
	`AMEND WHAT /COMPOSITION_SET/: <SUBJECT>`
	Several subjects for the phase can be amended but most often this command is used to enter two or more composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.
	Enter a question mark at the prompt to get a list of all possibly amended subjects for a phase.

There are no additional prompts for DEBYE_HUCKEL, HKF_ELECTROSTATIC, GLASS_TRANSITION, QUASICHEM_FACT00, QUASICHEM_ISRID, REMOVE_ADDITION, and DEFAULT_STABLE.	
`RENAME_PHASE`	`NEW PHASE NAME /ABCD/: <PHASE NAME>` Give a new phase name for the chosen phase, or press <Enter> to keep the default shown.
`SITE_RATIOS`	`SITES IN FIRST SUBLATTICE /XX/ : <YY> SITES IN SECOND SUBLATTICE /XX/ : <YY>` Specify the site numbers for each of the prompted sublattices for the current phase. Press <Enter> to accept the previous definitions.

`NEW_CONSTITUENT`	`SUBLATTICE /#/: <SUBLATTICE NUMBER>`
	Specify the sublattice where the new constituents are located.
	`SPECIES: <SPECIES NAME>`
	Give a valid species name.

`COMPOSITION_SETS`	`NEW HIGHEST SET NUMBER /#/: <SET NUMBER N>`
	The default value (#) is usually one higher than the current value. All phases have initially one composition set. If a lower value (i.e. lower than the default one) is given, that specific composition sets are deleted.
	You cannot take away the first composition set.
	`MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AB/: <MAJOR CONSTITUENT(S)>`
	Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept

Syntax	AMEND_PHASE_DESCRIPTION
	the default which was automatically set according to the specified composition set of the phase. This prompt is repeated for all available sublattices in the chosen phase. The major constituents in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

`MAJOR_CONSTITUENT`	`COMPOSITION SET /1/: <COMPOSITION SET NUMBER>`
	Give the composition set (digit number) for the chosen phase, or press <Enter> if you want to set major constituents for the specified composition set.
	`MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AB/: <MAJOR CONSTITUENT(S)>`
	Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept the default which is automatically set according to the specified composition set of the phase.
	This prompt is repeated for all available sublattices in the chosen phase for the specified composition set.
	The major constituents in each sublattice can be specified. This is useful in order to make calculations converge faster and more easily (because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set). The databases often set major constituents for several phases automatically when data are retrieved.

`FRACTION_LIMITS`	`ELEMENT : <EL1>`
	`LOW FRACTION LIMIT /0/ :  <APPROPRIATE LOW LIMIT>`
	`HIGH FRACTION LIMIT /1/ : <APPROPRIATE HIGH LIMIT >`
	`ELEMENT : <EL2>`
	`LOW FRACTION LIMIT /0/ :  <APPROPRIATE LOW LIMIT>`
	`HIGH FRACTION LIMIT /1/ : <APPROPRIATE HIGH LIMIT>`
	`ELEMENT : <ELN>`
	`LOW FRACTION LIMIT /0/ :  <APPROPRIATE LOW LIMIT>`
	`HIGH FRACTION LIMIT /1/ : <APPROPRIATE HIGH LIMIT >`

`MAGNETIC_ORDERING`	`THE ANTIFERROMAGNETIC FACTOR /XX/: <YY>`
	Specify the anti-ferromagnetic factor for the chosen phase. This should be –1 for BCC phase and –3 for all other phases (FCC, HCP, etc.).
	`SHORT RANGE ORDER FRACTION OF THE ENTHALPY /XX/: <YY>`

Syntax	AMEND_PHASE_DESCRIPTION
	The magnetic ordering is a second-order transformation and part of the enthalpy due to this transformation is due to short-range order. This value is the fraction of the total enthalpy that is due to short-range ordering above the magnetic transition temperature. The default value (xx) is 0.40 for BCC phase, and 0.28 for all other phases (FCC, HCP, etc.).
`DISORDERED_PART`	`DISORDERED PHASE NAME: <PHASE NAME>` Give the disordered phase name for which there is no ordering sublattice.

`EXCESS_MODEL`	`MODEL NAME /ABCDEFG/: <MODEL NAME>`
	The default model is the pre-set model for the solution phase, normally the REDLICH-KISTER_MUGGIANU model, or choose another model for the phase to be amended:
	• REDLICH-KISTER_MUGGIANU
	• REDLICH-KISTER_KOHLER
	• FLORY-HUGGINS POLYMER MODEL
	• MIXED-EXCESS-MODELS (R-K default)
	• HKF
	• PITZER
	• CENTRAL_ATOM_MODEL
	The MIXED-EXCESS-MODELS option has sub-options:
	`FIRST (THE INDEPENDENT) CONSTITUENT: <CONSTITUENT NAME>`
	`SECOND (THE DEPENDENT) CONSTITUENT: <CONSTITUENT NAME>`
	Specify the binary pair of constituents in the current substitutional solution phase (the first one as the so-called independent constituent, and the second one as the dependent constituent), for which you wish to change the binary excess model from the default REDLICH-KISTER model to another model (LEGENDRE or POLYNOM).
	You are repeatedly prompted with the first sub-option (i.e. `First (the independent) constituent` after you have specified the desired binary Excess model type. To make further changes of binary excess model for other specific binary pairs in the current substitutional solution phase, press <Enter> (implying that there are no more changes of binary excess model for all other possibly-remaining binary pairs that shall still use the default REDLICH-KISTER model).
	`EXCESS MODEL TYPE: /LEGENDRE/: <DESIRED BINARY EXCESS MODEL TYPE>`

Syntax	AMEND_PHASE_DESCRIPTION
	For the currently-specified binary pair, choose one the legal binary excess models: LEGENDRE, POLYNOM or REDLICH-KISTER. If the default binary excess model REDLICH-KISTER is used for a certain binary pair, you can either specify the model name (or in short as R-K) or press <Enter>. After this sub-option, it returns to the first sub-option *First (the independent) constituent:* either for further change(s) of binary excess model of any other binary pair(s) or for termination (by pressing <Enter>) in the MIXED-EXCESS-MODELS option.

`TERNARY_ EXTRAPOLAT`	`EXTRAPOLATION METHOD: /TOOP-KOHLER/: <TERNARY MODEL>`
	Choose a ternary extrapolation model for the current solution phase:
	• TOOP-KOHLER for Toop-Kohler Extrapolation Model
	• KOHLER-ALL for Kohler Extrapolation Model
	• MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model
	The TOOP-KOHLER option further prompts:
	`CONSTITUENT IN SUBLATTICE #: <BASIS CONSTITUENT NAME>`
	`FIRST INTERACTION CONSTITUENT: <INTERACTING CONSTITUENT NAME>`
	`TOOP CONSTITUENT: <TOOP CONSTITUENT NAME>`
	Specify the so-called Kohler constituents (entered as the basis constituent and first interacting constituent) and Toop constituent on a given sublattice in the current solution phase.

`QUASICHEM_ IONIC`	To use the Quasichemical Model for the chosen liquid phase, you must first enter it as an ionic liquid phase, and then use this amending option. It creates a completely new phase, the original IONIC_LIQUID phase remains in the system and is not changed. `NUMBER OF BONDS/ATOM /2/: <NUMBER OF BONDS PER ATOM>` Specify the Z value (number of bonds per atom).
`STATUS_BITS`	Correct the phase status bits. It is important to fully understand this command before using it: `NEW STATUS WORD (IN HEXADECIMAL) /04204000/: <NEW STATUS BITS>` Also see *LIST_STATUS* on page 80 for information on the status bits. Normally, these should never be changed in this way, because such phase status bits are automatically set on when all the phase descriptions (predefined in databases

Syntax	AMEND_PHASE_DESCRIPTION
	and amended in the GIBBS module) are defined properly. The only exceptions are for the Kapoor-Frohberg-Gaye cell model for liquid SLAG solution phase, which can be set only as 04208000; and for the complete Revised HKF AQUEOUS solution model, which can be set as `02084000`.

AMEND_SYMBOL

In the GIBBS and PARROT modules, interactively calculate the current values of a function or table (predefined by the switched database or previously entered with *ENTER_SYMBOL* on page 72) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.

The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with *LIST_STATUS* on page 80. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

Syntax	AMEND_SYMBOL

Prompts	`NAME: <SYMBOL NAME>`
	Specify the name of an entered symbol.
	For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the `Parameter` keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:
	`FUNCTION VALUE  2.52500000E+01`
	`TABLE VALUE  1.56000000E+02`
	For variables and functions (or parameters), there are additional prompts and depend on the symbol type.

	For a variable, its current value is displayed, and you can change it to a new value:
	`VALUE /CURRENT VALUE/: <NEW VALUE>`
	For a function (or a parameter entered as a symbol):
	`DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: <Y OR N>`
	To change the number of ranges for the function, or change some of the temperature limits in the definition, For `Y`, you must retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.
	If you do not want to change it, press <Enter> to accept the default. The definition of the chosen function in all ranges (if any) is listed, for example:
	`DIFFERENT FUNCTIONS IN THESE RANGES`
	`298.15<T<2000.00`
	`2000.00<T<4500.00`
	`4500.00<T<6000.00`
	and this message displays:
	`Do you want to change range limits /no/: <y or n>`
	If a function is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any change.

	`RANGE NUMBER (0 TO EXIT) /0/: <RANGE NUMBER>`
	`FUNCTION:`
	The previous function is available for editing. The editing is performed within the general

Syntax	AMEND_SYMBOL
	subroutine FOOLED. This routine prompts as follows: `1:+:>` The prompt consists of the current position in the string and the character at that position between colons (::). **Commands** These commands can be given: • Help: `?` • Move CP to last or first character: `<+/-> A` • Delete characters from CP: `<+-#characters> D` • Exit: `E` • Find: `<#occurrences> F<string>@` • Insert: `I<string>@` • Move: `<+-#positions> M` • Restore string: `R` • Substitute: `S<OLD>@<NEW>@` • Type string: `T` where `CP` denotes the current position in the string, # means number of, @ is a terminator of an input or search string. When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type `E` at the prompt.

CHANGE_STATUS

For the GIBBS_ENERGY_SYSTEM Module, the status of an element or species or phase can be either ENTERED or SUSPENDED. The suspended status can be either implicit or explicit. The implicitly suspended status can be set e.g. for a species if any of the elements in its chemical formula is explicitly suspended. A species that is implicitly suspended becomes entered automatically if all its elements are set entered. After this command, a message shows which elements/species/phases are suspended or restored (entered). Consequently, the status bits for the specified elements or species or phases are changed, as listed with *LIST_STATUS* on page 80.

Syntax	CHANGE_STATUS
Prompts	`FOR ELEMENT, SPECIES OR PHASE /SPECIES/: <KEYWORD>` Specify the keyword (`element`, `species` or `phase`).
	`SUSPEND /Y/: <Y OR N>` The status is changed from ENTERED to SUSPENDED (`Y`), or vice versa (`N`). If an element is suspended all species with this element become implicitly SUSPENDED too. A phase may become implicitly suspended if all its constituents or all constituents in a sublattice are suspended.
	`LIST OF ELEMENTS/SPECIES/PHASES: <NAME OF ELEMENTS OR SPECIES OR PHASES>` Specify the names or indices of those elements or species or phases that shall become suspended or active. For names, these should be separated by a space and terminated with a semicolon (;) or an empty line. For indices it is possible to give a range by separating two numbers by a hyphen (-). The list should be terminated by a semicolon (;). Example: `5 1 7-12 FE;`

ENTER_ELEMENT

Specify a system interactively. The program searches the currently switched or preset database for data for the given elements. The data for the elements in the database are the:

- mass in g/mol
- name of the Selected Element Reference State (SER) which normally is the stable phase for the element at 298.15 K
- enthalpy difference for the element in the SER state at 298.15 K and zero K
- absolute entropy for the element in the SER state at 298.15 K.

The two predefined elements, i.e. electrons and vacancies, have the chemical symbols `/-` and `VA`, respectively. Initially, these are suspended but can be entered either by this command or *CHANGE_ STATUS* on the previous page.

If an aqueous solution phase is involved, in the GIBBS module you enter a special aqueous electron called, ZE. This is specially designed for appropriately calculating the standard electric potential in the aqueous solution system.

Syntax	ENTER_ELEMENT
Prompt	`ELEMENT NAME: <ELEMENT NAME>` Specify several elements on one line. The name of an element is its chemical symbol. The chemical symbols must be separated by spaces. Fictitious element names are legal but naturally no data are found in the database for them.
	An element name (maximum 2 characters) can either have its first letter in upper and the second (if any) in lower case (i.e. Lower Case Mode) or both letters can be in upper or lower case (i.e. Upper Case Mode). The Upper or Lower Case Mode is selected by the command *REINITIATE* on page 83, which removes all data, and should be executed before any other command.

About the ENTER_PARAMETER Command

For the PARROT Module, this command is the same and is described here. Also see *ENTER_PARAMETER* on page 99 for the command details.

In the descriptions of the standard thermochemical properties and special physical properties for a phase, there are a number of parameters which may depend on the temperature and pressure. The expressions for these parameters can be given in a free form as a sum of terms with powers of T and P and may also include the natural logarithm and exponential function. This type of expression is called *TP-functions*. Identical parameters (in terms of parameter-names) are stored only once in the GIBBS workspaces.

The composition-dependence of the Gibbs energy is described in the GIBBS module by the internal data structure, which is created when the phase is entered (see *GIBBS_ENERGY_SYSTEM Commands* on page 42). The Gibbs energy of a phase is always referred to one formula unit of the phase, i.e. the amount derived from the number of sites (i.e. the stoichiometric coefficient) for each sublattice. If vacancy is a constituent of a sublattice, the amount of matter per formula unit of the phase may vary with composition.

Defining the Parameter

A valid parameter should have the general form of:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx> <expression> <yyy> <keyword
Y or N> <zzz> !
```

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis. The parameter form is defined as:

- `<identifier>` is the parameter type;
- `<phase>` is the phase name (maximum 24 characters);
- `<constituent array>` is the specific constituent array in the phase;
- `<digit>` is the degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted;
- `<expression>` is the mathematical relation to describe the parameter;
- `<xxx>` and `<yyy>` are the low and high temperature limits respectively for the applicable temperature range of the parameter expression;
- `<keyword Y or N>` is the indicator on if there is continuation for the parameter expression or not;
- `<zzz>` is the reference index/number for the assessment of this parameter;
- The exclamation point ! is used to indicate that the current parameter definition is ended.

PARAMETER NAME

The GES parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Examples of parameter names:

- `G(GAS,C1O2)`: The Gibbs energy of formation of a CO2 molecule in gas.
- `G(FCC,FE:VA)`: The Gibbs energy of formation of fcc Fe with interstitials.
- `L(LIQ,Fe,Cr;0`: The regular solution parameter for Fe and Cr in liquid.
- `L(LIQ,Fe,Cr;1)`: The sub-regular solution parameter.
- `TC(BCC,Fe:Va)`: The Curie temperature of bcc Fe.
- `BMAGN(BCC,Fe:Va)`: The Bohr magneton number parameter of bcc Fe.

The parameter name consists of several parts. The first is a type-identifier and these can be used:

- `G`: Standard energy parameter (Gibbs energy of formation) or for interaction parameters;
- `L`: Excess energy parameter (Gibbs energy of interaction) always used for interaction parameters;

- `TC`: Curie temperature for magnetic ordering;
- `BMAGN` or `BM`: Bohr magneton number for magnetic ordering (or Born function ωPr,Tr for aqueous solute species).
- `VO`: Molar volume at 298.15 K and 1 bar (a numeric value only);
- `VA`: Integrated thermal expansivity; $\int_{298.15}^{T} \alpha\,(T)\mathrm{d}T\int_{298.15}^{T} \alpha\,(T)\mathrm{d}T$
- `VB`: Bulk modulus at 1 bar;
- `VC`: Isothermal compressibility;
- `VK`: High-pressure fitting parameter.

When necessary quantities as `H` (enthalpy), `S` (entropy), `V` (Volume), `F` (Helmholtz energy), etc., can be calculated from the Gibbs energy.

PHASE NAME

Specifying the `PHASE NAME` in uppercase is recommended; however, if you prefer to write it as a mixture of uppercase and lowercase, it automatically converts all lowercase to uppercase, as the GIBBS module only recognises uppercase phase names. It is important that if a phase bears a legal phase-type (among `G`, `A`, `Y`, `L`, `I`, `F` and `B`) in its phase definition (already by the `PHASE` keyword; such as GAS:G, LIQUID:L,SLAG:L, IONIC-LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name when ENTER_PARAMETER is executed.

CONSTITUENT ARRAY

The constituent array consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents (as the following prompt).

Solution phases with sublattices can have interacting constituents in each sublattice.

INTERACTION PARAMETER

An interaction parameter, which is used to describe the excess term of a quantity, must have two or more constituents that interact with each other on a specified sublattice site of the given phase. It is arbitrary which of these constituents is given as the first constituent and what is given as the interacting constituents. The software always sorts the constituents (in each sublattice) in alphabetical order when the parameter name is written as a prompt (for entering its parameter value) and when the parameter is listed (using the GIBBS commands *LIST_PARAMETER* on page 102 or *LIST_PHASE_DATA (from GIBBS)* on page 103). This is important for all asymmetric interaction parameters where the sign of the interaction parameter must depend on the appearance order.

Use an asterisk* to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L(FCC_L12,AL,NI:*)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the `FCC_L12` solution phase, while it is independent of all constituents on the second sublattice. An interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk * is calculated with the term of [1∑y (specified constituents)], which implies that in an A-B binary system these `L` parameters are identical (but in higher-order systems, these are different):

- `L(phase,A,B)` is multiplied with X(A)*X(B)
- `L(phase,A,*)` is multiplied with X(A)*(1-X(A))
- `L(phase,B,*)` is multiplied with X(B)*(1-X(B))

If you press <Enter> when you are asked for a parameter name or if you have improperly input the entire parameter name, you are asked for each of these items in the name.

ENTER_PARAMETER

For the PARROT Module, this command is the same and is described here.

Also see *About the ENTER_PARAMETER Command* on page 95 for details about each of the options.

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command *AMEND_PARAMETER* on page 44.

Syntax	ENTER_PARAMETER

Prompts	`PARAMETER: <PARAMETER NAME>`
	As explained in *About the ENTER_PARAMETER Command* on page 95, specify a correct and complete `Parameter Name`, which should contain all the necessary parts of the general form:
	`<IDENTIFIER>(<PHASE>,<CONSTITUENT ARRAY>;<DIGIT>)`
	If a parameter name is not acceptable or <Enter>, is pressed, a message displays:
	`*** Error, please re-enter each part separately`
	and you are prompted for input for each required part for a parameter name.

Options	**Description or Information**
`IDENTIFIER`	`IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.
`PHASE NAME`	`PHASE NAME (/ABCD/): <PHASE NAME>` Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.
`CONSTITUENT`	`CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME>` A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated. It is the species name, not the stoichiometric formula required here. If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing <Enter> if the constituent is the same, or specify a new species name.
`INTERACTING CONSTITUENT`	For phases with several sublattices, the program asks for one constituent in each sublattice. `INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> to accept it if the constituent is the same, or specify a new species name.

Syntax	ENTER_PARAMETER
	To cancel the default value of the interacting constituent type `NONE` or the name of another constituent. This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an <Enter> is enforced.
`DEGREE`	`DEGREE /#/: <DEGREE>` Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (`L`), Curie temperature (`TC`) and Bohr magneton number (`BMAGN`), as well as for volume-related parameters (`V0`, `VA`, `VB`, `VC` or `VK`). For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index. For a standard `G` parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.

`PHASE PARAMETER`	After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.
	`LOW TEMPERATURE LIMIT /298.15/: <LOWEST TEMPERATURE LIMIT IN K>`
	Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	`FUNCTION: <DEFINITION FOR A FUNCTION>`
	A TP-Function consists of terms in T and P.
	`& <CONTINUATION OF THE DEFINITION FOR THE CURRENT FUNCTION>`
	Continuation of a TP-Function definition.
	`HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K>`
	Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the *lowest limit* is entered as a negative number) for the current TP-Function.
	`ANY MORE RANGES /N/: <Y OR N>`
	Enter `Y` for more function(s) or `N` to end this command.

About the ENTER_PHASE Command

With the command *ENTER_PHASE* on page 69 , the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces.

About Phase Names

A thermochemical system must have at least one phase (which is a homogeneous part of the system with a uniform composition and structure). In the GIBBS module, any number of phases can be entered for a system and for each phase there must be a description of how its Gibbs energy varies with temperature, pressure and composition. A phase has a large amount of data connected to it, e.g. it starts with a phase name:

- It may be treated as a special phase-type;
- It may have structural information about sublattice(s), etc.,
- There must be a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase);
- There may be basic information on what kind of EXCESS_MODEL (polynomial expression) is used to describe the binary, ternary and/or higher-order interactions between constituents;
- There may be so-called Additional contributions to the Gibbs energy of the phase from special physical phenomena, e.g. magnetic ordering, hypothetical electrostatic interaction, and so forth;
- There must exist all the parameters required for the descriptions of thermochemical properties (i.e. `G` terms for standard Gibbs energies, and `L` terms for binary, ternary or higher-order interaction excess energies) and of some special physical properties (e.g. the Curie temperature `TC` and Bohr magneton number `BMAGN` (or `BM`) for magnetic ordering, `V0`-`VA`-`VB`-`VC`-`VK` parameters for volume contributions, Born functions for hypothetical electrostatic interaction in an aqueous solution phase) stored in connection with the phase.

About Phase Type Code

A G phase (gaseous mixture) or an A phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and that an L phase (ordinary liquid solution) is normally (but not always) modelled as a substitutional phase without sublattice, too.

The F and B phase-types are useful for ordered FCC (or HCP) and BCC solution phases handled by the so-called Four Substitutional-Sublattice Ordering Model, which always requires that the solution phase must have four sublattices for substitutional ordering and can additionally have an interstitial sublattice.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices all of which are the nearest neighbours. A *Normal 4-Sublattice*

Model requires that all the G parameters for each of end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option F means that the G parameters need be given only once. The possible permutations are handled automatically. To be more clarified: An A-B binary solution phase (with the element A locates on one sublattice site and B on three sublattice sites) treated by the Normal 4-Sublattice Model has to have 4 G parameters for 4 end-members, i.e. G(phase,A:B:B:B), G (phase,B:A:B:B), G(phase,B:B:A:B) and G(phase,B:B:B:A), because of that in the general case these G parameters can be different from each other. But for the FCC and HCP orderings, these are identical and thus all G parameters of such end-members need be given only once, and the possible permutations are then automatically handled by the GIBBS module. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

There are restrictions on the excess parameters allowed with the phase-type option `F`. You can only have excess parameters of these types:

```
L(phase,A,B:*:*:*;0…9)
L(phase,A,B:C,D:*:*;0…9)
```

The asterisk * means that the interaction parameter is independent on the constituents on its corresponding sublattice. No ternary interaction parameters (i.e. with three elements on one sublattice site) are allowed. The reason for this restriction is that it would be too complicated to handle all possible permutations. In the current *Four Substitutional Sublattice Ordering Model*, the binary interaction between A and B atoms is thus independent of the constituents on the other sublattices, where there are many other parameters to model the composition-dependence of the Gibbs energy (both in the ordered and disordered parts of the phase). The model for these ordered phases are always partitioned in a disordered part (with a single substitutional sublattice) and an ordered part (with four substitutional sublattices for ordering).

For ordered BCC phases, the phase-type option B means the same thing but the situation is more complicated, as the 4-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase (with the element A locates on two sublattice site and B on other two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the G(phase,A:A:B:B) term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the G(phase,A:B:A:B) term has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds

For detailed reference visit the Crystal Lattice Structure web page http://www.nrl.navy.mil/mstd/branches/6390.

The first end-member (described by the G(phase,A:A:B:B) term) represents B2- ordering and the second (described by the G(phase,A:B:A:B) term) stands for B32-ordering. There are two permutations of the G (phase,A:A:B:B) term and four permutations of the G(phase,A:B:A:B) term, automatically conducted in the Four Substitutional-Sublattice Ordering Model. And there are also two kinds of reciprocal interaction parameters, i.e.

```
L(phase,A,B:C,D:*:*;0…9) L(phase,A,B:*:C,D:*;0…9)
```

An advanced feature with the phase-type options F and B is that a composition set that represents the solution phase has a suffix (indicating that it is really as an ordered or disordered phase) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams). Such suffix indications can be:

- `_L12` or `_L10` for ordered FCC
- `_A1` for disordered FCC
- `_B2`, `_B32`, `_D03` or `_L21` for ordered BCC
- `_A2` for disordered BCC
- `_D019` and `_B19` for ordered HCP
- `_A3` for disordered HCP

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
FCC PHASE	PHASE_A1	PHASE_L12
		PHASE_L10
BCC PHASE	PHASE_A2	PHASE_B2
		PHASE_B32
		PHASE_D03
		PHASE_L21
HCP PHASE	PHASE_A3	PHASE_D019
		PHASE_B19

ENTER_PHASE

See *About the ENTER_PHASE Command* on page 67 for details about the phase-type and other prompts.

With this command, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces. However, for the remaining parts of thermodynamic descriptions (i.e. thermochemical and physical parameters, excess model, and possibly additional contribution term) for the phase, the GIBBS commands *ENTER_PARAMETER* on page 99 and *AMEND_PHASE_DESCRIPTION* on page 52, should be used sequentially.

Normally, data for a system are retrieved from the preset database after the elements and species are specified. This is automatically done through *GET_DATA* on page 15. In some cases, specify a phase interactively.

Syntax	ENTER_PHASE
Options	**Description and Information**

`PHASE NAME`	`NAME OF PHASE: <PHASE NAME>`
	The phase name is any string starting with a letter and containing only letters, digits or the underscore character. The phase name must be unique.
	`TYPE CODE: <PHASE-TYPE CODE>`
	The `Phase-type code` must be specified for the phase if it is not an ordinary solution phase. Press <Enter> if the phase is ordinary.

`PHASE-TYPE`	
`G`	Gaseous mixture phase. There may only exist one gas phase in a system.
`A`	Aqueous solution phase.
`L`	Liquid solution phase but not `A` (aqueous) or `Y` (ionic liquid)
`Y`	Ionic liquid solution phase (that is specially treated by the Ionic Two Sublattice Liquid Model).
`I`	A phase with charged species but not `G` (gaseous), `A` (aqueous) or `Y` (ionic liquid).
`F`	An ordered FCC or HCP solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).
`B`	An ordered BCC solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).

`SUBLATTICE NUMBER`	`NUMBER OF SUBLATTICES /1/: <SUBLATTICE NUMBER>`
	Phases with stoichiometric constraints usually have two or more sublattices. On each sublattice one or more species can be entered as constituents. The number of sublattices must not exceed 10. Substitutional phases with no sublattices are treated as phases with one sublattice.
	`NUMBER OF SITES ON SUBLATTICE # /1/: <SITE NUMBER>`
	For phases with sublattices, the ratio of the sites on each sublattice (donated with #) must be given. The program asks for values for all sublattices (by repeating this question for each sublattice), but these may have a common factor extracted. It is

Syntax	ENTER_PHASE
	recommended to use integer numbers as sites if possible. For substitutional phases with no sublattices, this question does not show up.

`CONSTITUENTS`	`NAME OF CONSTITUENT: <CONSTITUENT NAME(S)>`
	For each sublattice specify at least one species as constituent. Several constituents can be given consequently (on the repeated prompt) or on the same line separated by a space. This question is repeated till pressing <Enter> or giving a semi-colon (;), meaning that the list of constituents is terminated by (;) or an empty line.
	`WILL YOU ADD CONSTITUENTS LATER /NO/: <Y OR N>`
	For `Y` add other constituents to the phase by specifying new components in e.g. an ENTER_PARAMETER command. The default is `N` or press <Enter>.
	If illegal constituents are used, you get a message e.g. when parameters are entered.
	`DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: <Y OR N>`
	Enter `Y` for a list of all possible parameters up to the fifth interaction order for the entered phase.

ENTER_SPECIES

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. For each species, its name and chemical formula must be given.

All elements are automatically entered simultaneously as species. The constituents of a phase must be species, but there is no thermochemical data associated with the species except as constituents of a phase.

Syntax	ENTER_SPECIES

Prompt	`SPECIES NAME: <SPECIES NAME>`
	Enter a unique species name. This is usually its chemical formula but it can be any string which starts with a letter and contains only letters or digits. Parenthesis () and an underscore _ are permitted. The combination /- or /+ used to denote charge.
	Species Names Examples
	`NACL2, FE2O3, FEO3/2, FE1O1.5, CA.5MG.5SI1O3,`
	`AL1H1O1_Al(OH) , AL1H1O1_HAlO, C2H4O3_124TRIOXOLANE, NA+, SIO4-4, H1/+1, H1O1/-1, AGC2N2-1.`
	The species name can be used to separate isomers with the same stoichiometry, e.g. `C2H2Cl2, (CHCl)2_cis, (CHCl)2_trans, CH2_CCl2.`

	`STOICHIOMETRY /SPECIES NAME/: <CHEMICAL FORMULA>` The elements in the chemical formula are normally separated by stoichiometric numbers. Neither parenthesis () nor an underscore _ is allowed in the chemical formula, while the special combination /- or /+ can be used. In upper case mode (see *REINITIATE* on page 83), the stoichiometric number unity can be excluded only if the element symbol consists of two letters. In lower case mode, the element must be typed with the first letter in UPPER case and the second in lower, and it is thus possible to distinguish CO (carbon monoxide) from Co (cobalt) without any stoichiometry number. All elements in a species must be entered prior to entering the species.

ENTER_SYMBOL

The information about this command is specific to the Thermo-Calc GIBBS module in Console Mode.

In the GIBBS module, a symbol can be used to represent a numeric quantity (e.g. a *variable*), a *function*, or a *table*. The entered symbol (with a symbol name of maximum eight characters) can be used later when parameters are entered, and this is a flexible way to manipulate thermodynamic functions. Symbols are especially useful if the same function or table is used in several thermochemical parameters. A *parameter* symbol is used to assign the values of phase parameters (which are defined with the command *ENTER_PARAMETER* on page 99) to specific characterized symbols. If you want to define a constant quantity, enter it as a simple function with a constant value in all (temperature) ranges.

The symbols entered in the GIBBS module can also be listed and used in the *PARROT Commands* on page 86 (for data optimization) where you can use the GIBBS-entered symbols (variables, functions or parameters) to define parameters that shall be optimized.

Symbols entered in the GIBBS module are not the same symbols as defined in the POLY and POST modules.

Also see *ENTER_SYMBOL* on page 195 for the POLY and POST modules.

See example 44 in the *Console Mode Examples Guide*for an example of using variables and functions.

Syntax	ENTER_SYMBOL

Prompt	`VARIABLE, FUNCTION, TABLE OR PARAMETER? /FUNCTION/: <KEYWORD>`
	The `keyword` can be a variable, function, table or parameter.
	• `Variables` are similar to functions because these can also be expressions of state variables. It is possible to enter a variable with a new expression anytime.
	• `Functions` are expressions of state variables or other functions.
	• `Tables` are used for listing results. A table consists of a list of any number of state variables, functions or variables.
	• `Parameter` symbols are used to assign the values of phase parameters (which are defined by the command ENTER_PARAMETER) to specific characterized symbols. If the phase parameter is not defined yet, the parameter symbol is assigned zero or a symbol which is valued as zero. In this way it is easy to refer to entered phase parameters in further defining other phase parameters.
	`NAME: <NAME OF THE SYMBOL>`
	Each symbol has a unique name that must start with a letter and can have maximum 8 characters.
	The following prompts are based on the type of symbol.

`Variable` symbol	`VALUE: <NUMERIC VALUE OF A VARIABLE>` Only a constant numeric value, not an expression, is accepted.
`Function`	Enter the lower-temperature limit, the expression, an upper-temperature limit and if

Syntax	ENTER_SYMBOL

symbol	there is another expression above this upper limit:
	`LOW TEMPERATURE LIMIT /298.15/: <LOWEST TEMPERATURE LIMIT IN K>`
	Specify the lowest-temperature limit, below which its (first) expression is not applicable. The default lowest limit of all kinds of data is 298.15 K.
	If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this function; in such a case, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function are also taken as pressure limit values (in Pascal).
	The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-FUNCTIONS valid in the nearest temperature/pressure range.
	`FUNCTION: <DEFINITION FOR A TP-FUNCTION>`
	A TP-Function consists of terms in T and P. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. An expression can be continued on more than one line. A PT-function must be terminated by a semicolon (;) or an empty line. No more than 78 characters can be written on a line. If this is not sufficient space on one line, press <Enter> and continue on the next line. The program prompts with an ampersand `&` when a continuation is expected.
	A function can have several temperature ranges, and a different expression (i.e. a TP-Function) for each region; if required, a single function can have up to ten different temperature ranges (and thus have up to ten different TP-Functions).
	This question is repeated if the current function has more than one expression (TPFunction) in various temperature ranges [or pressure ranges; only if the *lowest limit* is entered as a negative number)].
	`& <CONTINUATION OF THE DEFINITION FOR THE CURRENT TP-FUNCTION>`
	This is for a continuation of the definition for the current TP-Function. The ampersand & means that you can continue to write the function on the new line if one line is not enough for the current TP-Function. If you are finished the current TP-Function, press <Enter> again.

Syntax	ENTER_SYMBOL

	`HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K>`
	For a TP-Function, specify the high-temperature limit, above which its current expression is not applicable. The default high-temperature limit for all kinds of data is always 6000 K.
	This question is repeated if the function has more than one expression (TPFunction) in various temperature ranges.
	All the temperature limits for the presently-be-entered TP-Function MUST be in an increasing order; otherwise the whole function is given a single value of zero.
	If a negative number is given as the lowest-temperature limit, it is interpreted as the low-pressure limit (in Pascal), and the high-temperature limit is also taken as the high-pressure limit (in Pascal) for the current TP-Function.
	The high-temperature/pressure limit for the current applicable expression (TPFunction) is the low temperature/pressure limit for the next range if several ranges are needed to describe the temperature/pressure-dependence of this function.
	The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-Function valid in the nearest temperature/pressure range.
	`ANY MORE RANGES /N/: <Y OR N>`
	Answer `N` to finish the definition of the current function. If `Y` the program asks for a new function valid above the last high temperature limit and below a new high temperature limit. The maximum number of temperature ranges is 10.
	Important note: Make sure that the function and its first derivatives are continuous across break points.

`Table` symbol	Specify the low and high temperature limits, temperature step and tabled value at each specified temperature:
	`LOW TEMPERATURE LIMIT /298.15/: <LOW TEMPERATURE LIMIT IN K>`
	The lowest temperature where the table has a value.
	`HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K>`
	The highest temperature where the table has a value.

Syntax	ENTER_SYMBOL

	`STEP IN TEMPERATURE /100/: <TEMPERATURE STEP>`
	The step in temperature between each value in the table. This step must be constant for the whole table. If a table cannot be described with a single step it must be divided into several tables for different temperature ranges. The upper and lower limits are truncated to give reasonable values where the table values must be specified.
	`TABLE VALUE AT  XX /YY/: <TABLE VALUE>`
	The value of the table at the specified temperature (`xx`) must be given. The default value (`yy`) is the last value.

`Parameter` symbol	Input the correct name of a phase parameter (including its identifier, phase name, constituent and interacting constituent(s) in various sublattices (if exist), and degree of the parameter. Most of the settings are the same as in the *ENTER_PARAMETER* on page 99 command or the Function symbol prompts above.
	`PARAMETER: <PARAMETER NAME>`
	Specify a correct and complete parameter name, which should contain all the necessary parts of the general form:
	`<IDENTIFIER>(<PHASE>,<CONSTITUENT ARRAY>;<DIGIT>)`
	If a parameter name is not acceptable or <Enter> is pressed, this error message displays:
	`*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY`
	The program prompts for separate input for each required part for a parameter name.
	`IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK>`
	Specify one of these types of legal identifiers.
	`PHASE NAME (/ABCD/): <PHASE NAME>`
	Specify the phase name.
	`CONSTITUENT (IN SUBLATTICE  # /ABC/): <SPECIES NAME>`
	Specify the constituent name on the specified sublattice site of the given phase.
	`INTERACTING CONSTITUENT (IN SUBLATTICE  # /XYZ/): <SPECIES NAME>`
	Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	`INTERACTING CONSTITUENT (IN SUBLATTICE  # /XYZ/): <SPECIES NAME>`
	If there is more than one interacting constituent on the specified sublattice site of the

Syntax	ENTER_SYMBOL

	given phase, specify them; otherwise press <Enter>.
	`DEGREE /#/: <DEGREE>`
	Specify an integer number (a value from 0 through 9) as the degree for the phase parameter.
	`LOW TEMPERATURE LIMIT /298.15/: <LOWEST TEMPERATURE LIMIT IN K>`
	Specify the lowest-temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	`FUNCTION: <DEFINITION FOR A FUNCTION>`
	Specify the desired TP-Function for the current temperature range (or current pressure range; only if the *lowest limit* is entered as a negative number).
	`& <CONTINUATION OF THE DEFINITION FOR THE CURRENT TP-FUNCTION>`
	Specify the desired TP-Function continuation for the current temperature range (or current pressure range; only if the lowest limit is entered as a negative number).
	`HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K>`
	Specify the high-temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the lowest limit is entered as a negative number) for the current TP Function.
	`ANY MORE RANGES /N/: <Y OR N>`

LIST_CONSTITUENT

Syntax	LIST_CONSTITUENT
	List all the constitutions (as site-fractions) for all the phases in the defined system.
	📝 This is mainly for software managers. There are no commands in the GIBBS monitor to set the constitution.

LIST_DATA

All data for the current system that is defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) within the current GIBBS workspace is written in a readable manner on the output file. If no output file is specified, the data display on screen.

The output data consists of a list of all elements and their data followed by a list of all phases and the data associated with each phase. The thermochemical parameters listed for each phase are always in SI units.

For encrypted commercial databases you may not be able to use this command to list any retrieved data. However, it can be used to list some basic definitions (such as phase models and phase-constituents) retrieved from an encrypted database, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

Syntax	LIST_DATA
Prompts	`OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME>` Specify the name of a file in which the data shall be written in a readable manner. The default value is the screen (by pressing <Enter>).
	`OPTIONS?: <OPTION(S)>` Choose one or several of these options for output: • `N` the output is written as a user database format. • `P` the output is written as a macro file for future input. This is useful for creating `*SETUP` files for data assessments. • `S` the symbols are suppressed. • `R` the references for the parameters are listed (only for some databases in which references are available) • `L` the output is written suitable for a LaTeX preprocessor.

LIST_PARAMETER

This command is for both the GIBBS and PARROT modules.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

```
THE PARAMETER NAME: <IDENTIFIER>(<PHASE>,<CONSTITUENT ARRAY>;<DIGIT>)
```

For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

Syntax	LIST_PARAMETER

Prompts	`PARAMETER: <PARAMETER NAME>`
	Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)
	See *About the ENTER_PARAMETER Command* on page 95 to learn how to define the Parameter Name.
	If a parameter name is not acceptable or <Enter> is pressed, an error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each required part for a parameter name.

	`IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK>` Specify one of these types of legal identifiers.
	`PHASE NAME (/ABCD/): <PHASE NAME>` Specify the phase name.
	`CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME>` Specify the constituent name on the specified sublattice site of the given phase.
	`INTERACTING CONSTITUENT (IN SUBLATTICE  # /XYZ/): <SPECIES NAME>` Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	`INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME>` If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.
	`DEGREE /#/: <DEGREE>` Specify a numerical number as the degree for the phase parameter.

LIST_PHASE_DATA

All data for a specific phase are written in a readable manner on screen. The thermochemical parameters listed for the phase are always in SI units.

For encrypted commercial databases you may not be able to use this command to list any phase data. However, this command can be used for listing some basic definitions (such as phase model and phase-constituents) for the specified phase, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

Syntax	LIST_PHASE_DATA
Prompt	`PHASE NAME: <PHASE NAME>` Specify a phase name (if abbreviated, it should be unique).

LIST_STATUS

Syntax	LIST_STATUS
	For the GIBBS module, list the entered elements, phases and species with the status word. The command is included for system managers. Each element, species, phase and symbol has a set of status bits. The values of these bits are listed with this command. The bits are listed as hexadecimal, i.e. four bits are written as a hexadecimal number. Two hexadecimal numbers make a byte. In hexadecimal, 0 to 9 mean normal digits. A to F means values 10 to 15. The number `E4000000` has thus bit 1, 2, 3 and 6 equal to one. The bits are numbered starting with 1 for the most significant (leftmost) bit.

Element Status Word

Set the element status word (*Bit. Meaning*) if:

1. Element cannot be deleted (only vacancy and electron)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (cannot occur for an element)

Species Status Word

Set species status word (*Bit. Meaning*) if:

1. Species record for an element (each element has a species record)
2. Suspended (inclusive OR of bit 3 and 4)

3. Explicitly suspended
4. Implicitly suspended (e.g. if a species element is suspended)
5. Charged (inclusive OR of bit 6 and 7)
6. Negative charge
7. Positive charge
8. Vacancy
9. Component (by default the elements are the components)

Phase Status Word

Set phase status word (*Bit. Meaning*) if:

1. Ideal (no sublattices and no excess parameters)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (e.g. if all constituents suspended)
5. Gas phase
6. Liquid phase
7. Solution phase
8. Only one constituent (in each sublattice)
9. Ions (inclusive OR of bit 10 and 12)
10. New ionic liquid model (charge balance handled internally)
11. Constituents cannot be added
12. External charge balance needed
13. Aqueous model
14. Charged species (ions)
15. Dilute entropy
16. Last calculation exceeded temperature range for any parameter
17. Kapoor-Frohberg-Gaye cell model
18. Turbo calculation used
19. Turbo calculation impossible
20. Turbo calculation illegal

21. Phase is not ideal
22. Current site fractions saved
23. This phase is the ordered part
24. This phase is the disordered part (bit 2 and 3 also set)
25. Shadow phase with diffusion data
26. Error in ionic model
27. Sometimes
28. CVM-SRO (short-range ordering) entropy expression
29. CVM initialization is made
30. Used to test quasi-chemical ordering model
31. Major constituents check even if no miscibility gap (ordering)
32. Hoch-Arpshofen model

Symbol Status Word

Set symbol status word (*Bit meaning*) if:

1. Constant
2. Variable
3. Function
4. Table
5. Value must not be amended
6. Undefined

LIST_SYMBOL

List the symbols available in the current GIBBS workspace, which are defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) and used in TP-functions for the entered model parameters for various phases in the defined system.

For encrypted commercial databases you may not be able to use this command to list any retrieved symbol.

Syntax	LIST_SYMBOL
Prompts	`NAME: <SYMBOL NAME>` Specify a symbol name (either as the full name of a defined symbol, or as the first few common characters of several symbols which have names starting with such common characters). Only those symbols that match this name are listed. Or press <Enter> for a list of all the symbols defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) for the current system, which are available in the current GIBBS workspace.
	`OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME>` Specify the name of a simple-textual file in which the entered symbols shall be written in a readable manner (such a basic textual file can later on be opened and edited by any text editor). The default value is the screen (by pressing <Enter>).

READ_GES_WORKSPACE

The data area saved onto a *.GES5 file with *SAVE_GES_WORKSPACE* on the next page is read back into the GIBBS workspace.

Syntax	READ_GES_WORKSPACE
	Enter a **File name** and specify the working directory where to save the file in the **Look in** field. Normally the default file-type in the **Files of type** field is the correct one for the GIBBS workspace format (i.e. *.GES5 file). The saved *.GES5 files are unique for each CPU type, and therefore a *.GES5 file saved on one CPU type cannot be read and used on another CPU type.

REINITIATE

All data in the stored GIBBS workspace are erased, and all variables are initiated to their default values.

Syntax	REINITIATE
Prompts	`UPPER CASE ONLY /Y/: <Y OR N>` The name of elements and species can be either in only UPPER case (by typing `Y` or pressing <Enter>), or the elements with two letter names have the first letter in Upper and the second in lower case (by typing `N`). In upper case mode all input in lower case is automatically converted to upper case.
	`LOWER TEMPERATURE LIMIT /298.15/: <LOWEST T IN K>` This value is used as the lower temperature limit when data are entered interactively.
	`UPPER TEMPERATURE LIMIT /6000/: <HIGHEST T IN K>` This value is used as the upper temperature limit when data are entered interactively.
	`DEFAULT ELEMENT REFERENCE STATE SYMBOL INDEX /1/: <1 OR 2 OR 3>` Specify a proper index for the default listing parameters (symbol), or press <Enter> to accept the preset index 1. The *index* is for defining the symbol printed in listings of parameters. The symbol can be: - `G`: the data are referred to Gibbs energy at a variable temperature (also called *Lattice Stability*). - `H298`: the data are referred to the enthalpy of the element at 298.15 K and 1 bar. - `H0` is the same as H298 but at the temperature 0 K. The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data must you set the index to get the correct symbol. Set the index value to 0 to get the symbol `G`, to 1 to get the symbol `H298` and to 2 to get `H0`.

SAVE_GES_WORKSPACE

The data area used by the GIBBS workspace can be saved on a file (with a default extension GES5 under MS-Windows, or ges5 under Linux). The default file name is RESULT.GES5 or equal to the one used in a previous *READ_GES_WORKSPACE* on the previous page command.

Syntax	SAVE_GES_WORKSPACE
	Enter a **File name** and specify the working directory where to save the file in the **Save in** field. Normally the default file-type in the **Files of type** field is the correct one for the GIBBS workspace format (i.e. *.GES5 file). The output is unformatted and cannot be printed.

SET_R_AND_P_NORM

The value of the gas constant (R) is used to define the energy units that are used for input of data. On output, all data are in SI units. The value of the pressure 1 atm is used to interpret values of the pressure given by application programs.

Syntax	SET_R_AND_P_NORM
Prompts	`VALUE OF GAS CONSTANT IN YOUR ENERGY UNITS /8.31451/: <NEW VALUE>` The default value of the gas constant is in SI units (i.e. 8.31451). If you change this value, it only affects the interpretation of energy data given interactively from the terminal, e.g. if the value is set to 1.98717 you can give values in Calories.
	`VALUE OF ONE BAR IN YOUR PRESURE UNITS /100000/: <NEW VALUE>` The value of the pressure given in application programs is divided by this value and then multiplied with the value of one bar expressed in Pascal before it is used inside the GIBBS module.

PARROT Commands

In this section:

AMEND_PARAMETER

Interactively modify the TP-function(s) for a specific parameter for a phase with this command. This is useful in order to correct typing errors because the old function is made available for interactive editing on the terminal.

This AMEND_PARAMETER command is for the PARROT module. There is also a GES module command with the same name (*AMEND_PARAMETER* on page 44).

Syntax	AMEND_PARAMETER

Prompts	`PARAMETER: <PARAMETER NAME>`
	Specify a correct parameter name. If a parameter name is not acceptable or <Enter> is pressed, the error message displays:
	`*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY`
	The program prompts for separate input for each part for a parameter name.

	`IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK>` Specify one of these types of legal identifiers (see *ENTER_PARAMETER* on page 99).
	`PHASE NAME (/ABCD/): <PHASE NAME>` Specify the phase name.
	`CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME>` Specify the constituent name.
	`INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME>` Specify the interacting constituent name; if there is no interacting constituent, press <Enter>.
	`INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME>` If there is more than one interacting constituent, specify these; otherwise press <Enter>.
	`DEGREE /#/: <DEGREE>` Specify a numerical number as the degree of the phase parameter.
	After the parameter name is specified correctly, the program lists its current definition (either preset in database or defined by the ENTER_PARAMETER command), such as:

```
L(PHASE2,AL,MG;1)=
298.15<T<2000.00: +5000
2000.00<T<4500.00: +4500
```

Syntax AMEND_PARAMETER

```
  4500.00<T<6000.00: +4000
```

You are prompted to change the parameter definition:

```
DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: <Y OR N>
```

To change the number of ranges for the chosen function, or change some of the temperature limits in the definition, by typing `Y` you have to retype both the low/high temperature limits and functions

If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press <Enter> to accept the default `N` the whole definition of the chosen parameter in all ranges (if any) is listed such as:

```
  DIFFERENT FUNCTIONS IN THESE RANGES

  298.15<T<2000.00

  2000.00<T<4500.00

  4500.00<T<6000.00
```

This message prompts:

```
DO YOU WANT TO CHANGE RANGE LIMITS /NO/: <Y OR N>
```

If there is more than one range, this question is prompted. Press <Enter>.

```
RANGE NUMBER (0 TO EXIT) /0/: <RANGE NUMBER>
```

If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any change.

```
FUNCTION
```

The previous function is available for editing. The editing is performed within the general subroutine `FOOLED`, as described in *AMEND_SYMBOL* on the next page. This routine prompts as follows:

```
1:+:>
```

The prompt consists of the current position in the string and the character at that position between colons, (::).

Commands

These commands can be given:

- Help: `?`
- Move CP to last or first character: `<+/-> A`

Syntax	AMEND_PARAMETER
	- Delete characters from CP: `<+-#characters> D` - Exit: `E` - Find: `<#occurrences> F<string>@` - Insert: `I<string>@` - Move: `<+-#positions> M` - Restore string: `R` - Substitute: `S<OLD>@<NEW>@` - Type string: `T` where CP denotes the current position in string, # means number of, @ is a terminator of an input or search string. When the string is typed the character at the current position is replaced by an underscore `_`. To finish the editing of the current function, type `E`.
	`RANGE NUMBER (0 TO EXIT) /0/: <RANGE NUMBER>` Give a range number to edit that function, or press <Enter> or type `0` to exit this command.

AMEND_SYMBOL

In the GIBBS and PARROT modules, interactively calculate the current values of a function or table (predefined by the switched database or previously entered with *ENTER_SYMBOL* on page 72) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.

The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with *LIST_STATUS* on page 80. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

Syntax	AMEND_SYMBOL

Prompts	`NAME: <SYMBOL NAME>`
	Specify the name of an entered symbol.
	For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the `Parameter` keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:
	`FUNCTION VALUE  2.52500000E+01`
	`TABLE VALUE  1.56000000E+02`
	For variables and functions (or parameters), there are additional prompts and depend on the symbol type.

	For a variable, its current value is displayed, and you can change it to a new value:
	`VALUE /CURRENT VALUE/: <NEW VALUE>`
	For a function (or a parameter entered as a symbol):
	`DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: <Y OR N>`
	To change the number of ranges for the function, or change some of the temperature limits in the definition, For `Y`, you must retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.
	If you do not want to change it, press <Enter> to accept the default. The definition of the chosen function in all ranges (if any) is listed, for example:
	`DIFFERENT FUNCTIONS IN THESE RANGES`
	`298.15<T<2000.00`
	`2000.00<T<4500.00`
	`4500.00<T<6000.00`
	and this message displays:
	`Do you want to change range limits /no/: <y or n>`
	If a function is different in two or more temperature ranges, you must specify the range of

<table>
<tr><th>Syntax</th><th>AMEND_SYMBOL</th></tr>
<tr><td></td><td>the function of which you want to amend. Or press <Enter> or type <code>0</code> to exit this command without making any change.</td></tr>
<tr><td></td><td>
<code>RANGE NUMBER (0 TO EXIT) /0/: <RANGE NUMBER></code>
<code>FUNCTION:</code>
<p>The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:</p>
<code>1:+:></code>
<p>The prompt consists of the current position in the string and the character at that position between colons (::).</p>
<h4>Commands</h4>
<p>These commands can be given:</p>

Help: <code>?</code>
Move CP to last or first character: <code><+/-> A</code>
Delete characters from CP: <code><+-#characters> D</code>
Exit: <code>E</code>
Find: <code><#occurrences> F<string>@</code>
Insert: <code>I<string>@</code>
Move: <code><+-#positions> M</code>
Restore string: <code>R</code>
Substitute: <code>S<OLD>@<NEW>@</code>
Type string: <code>T</code>

<p>where <code>CP</code> denotes the current position in the string, # means number of, @ is a terminator of an input or search string.</p>
<p>When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type <code>E</code> at the prompt.</p>
</td></tr>
</table>

COMPILE_EXPERIMENTS

The descriptions of the experimental equilibria saved on a textual *.POP file, given as commands in the POLY and ED_EXP syntax, is compiled by this command into the PARROT structured data, i.e. stored into the current work *.PAR file which is created with *CREATE_NEW_STORE_FILE* on the next page, set by *SET_STORE_FILE* on page 116 , or opened with *READ_PARROT_WORKSPACES* on page 109, all done before COMPILE_EXPERIMENTS.

This command also lists the compilation details on screen or onto a listing file (*.TXT).

If a syntax error in the commands is detected, the compilation is terminated. You need to correct the error in the *.POP file (using a textual editor) and recompile it with the *.PAR work (store) file.

After a successful compilation, the program translates all the experimental data points in the *.POP file into a graphical experimental data file (*.EXP) in the DATAPLOT syntax, which can be further edited and used as a graphical experimental data file (*.EXP) for the purposes of imposing onto calculated/plotted phase diagrams and/or property diagrams for comparisons during the assessment process.

Also see the *DATPLOT User Guide* included with this documentation set.

Syntax	COMPILE_EXPERIMENTS
	A window displays to open the original experimental data file (*.POP). Enter a *.POP **File name** box, and specify the working directory in the **Look in** box. Normally the default file-type in the **Files of type** field is the correct one for the experimental data format (i.e. *.POP file). Click **Open** or **Cancel** button as applicable.
Prompts	`OUTPUT TO SCREEN OR FILE /SCREEN/: <*.POP FILE NAME>` A list of the source code in the *.POP file and error messages during compilation is written on screen (by pressing <Enter>) or on a list *.TXT file under a specific file name which can later on be opened and edited by any basic textual editor.
	`INITIATE STORE FILE /Y/: <Y OR N>` After a successful compilation, the data in the POLY3 workspace is stored as a new block of equilibria on the current work (store) file. If you specify that the store file should be initiated before compilation (`Y`), only the compiled block is stored on the current work file (consequently, the *.PAR file is updated). If a negative answer (`N`) is chosen here, the current work file is not changed. A window displays to generate/store the graphical experimental data file (*.EXP) in the DATAPLOT syntax. Enter a *.EXP file name in the **File name** field and specify the working directory when opening the *.EXP file in the **Look in** field. Normally the default file type in the **Files of type** field is the correct one for the graphical experimental data format (i.e. *.EXP file). Click **Open** or **Cancel** as applicable.

CONTINUE_OPTIMIZATION

This command continues the optimization using the same Hessian matrix.

In some cases it is not possible to attempt continuation. For example, if the optimization has already converged or if the optimizing parameters or the set of experimental equilibria used in the current optimization runs are changed. The program gives a warning message if you try to continue when you make these changes.

Syntax	CONTINUE_OPTIMIZATION

Prompts	`ARE YOU SURE? /N/: <N OR Y>`
	Prior to this question, a message displays to confirm if it is OK to continue:
	`It is safe to CONTINUE only after TOO MANY ITERATIONS  and no change in variables and experiments ...`
	You can accept the default (`N`) in order to cancel this special attempt.

	`NUMBER OF ITERATIONS /N/: <INTEGRAL NUMBER OF ITERATION>` Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT program tries this exact number of different sets of values of the optimizing variables without stopping the optimization even it would have converged earlier or should give up earlier.

CREATE_NEW_STORE_FILE

This file is hardware dependent and cannot be read by any text editor.

Create a binary file to be used as a *work file* (also called *store file*) before any optimization can be done. The workspace used by the GIBBS, POLY and PARROT modules is stored automatically on the work file but not any experimental information. The binary work file has a default extension of `PAR` under MS-Windows or `par` under Linux/UNIX.

A work file that is created at a previous run can be used in the PARROT module with the other command SET-STORE-FILE.

Syntax	CREATE_NEW_STORE_FILE
Prompt	<*.par file name> A **Save** window displays. Enter a **File name** and specify the working directory in the **Save in** field. Normally the default file-type in the **Files of type** field is the correct one for the PARROT workspace format (i.e. PAR file). Click **Save** or **Cancel** as applicable.

EDIT_EXPERIMENTS

Initialise and make available the sub-module for editing experimental equilibria, i.e. the ED_EXP module. All experimental equilibria compiled from the *.POP file can be accessed in the ED_EXP module.

The ED_EXP module is similar to the normal POLY module, but some commands are special and some POLY commands are not available. In the ED_EXP module, you can calculate each equilibrium separately or together, provide start values for equilibria which failed to converge, set weights, and modify the values of experiments or conditions.

Also see *Running the EDIT_EXPERIMENTS Command* on page 23.

Syntax	EDIT_EXPERIMENTS
	You are now in this submodule and can start using the commands.

About the ENTER_PARAMETER Command

For the PARROT Module, this command is the same and is described here. Also see *ENTER_PARAMETER* on page 99 for the command details.

In the descriptions of the standard thermochemical properties and special physical properties for a phase, there are a number of parameters which may depend on the temperature and pressure. The expressions for these parameters can be given in a free form as a sum of terms with powers of T and P and may also include the natural logarithm and exponential function. This type of expression is called *TP-functions*. Identical parameters (in terms of parameter-names) are stored only once in the GIBBS workspaces.

The composition-dependence of the Gibbs energy is described in the GIBBS module by the internal data structure, which is created when the phase is entered (see *GIBBS_ENERGY_SYSTEM Commands* on page 42). The Gibbs energy of a phase is always referred to one formula unit of the phase, i.e. the amount derived from the number of sites (i.e. the stoichiometric coefficient) for each sublattice. If vacancy is a constituent of a sublattice, the amount of matter per formula unit of the phase may vary with composition.

Defining the Parameter

A valid parameter should have the general form of:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx> <expression> <yyy> <keyword
Y or N> <zzz> !
```

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis. The parameter form is defined as:

- `<identifier>` is the parameter type;
- `<phase>` is the phase name (maximum 24 characters);
- `<constituent array>` is the specific constituent array in the phase;
- `<digit>` is the degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted;
- `<expression>` is the mathematical relation to describe the parameter;
- `<xxx>` and `<yyy>` are the low and high temperature limits respectively for the applicable temperature range of the parameter expression;
- `<keyword Y or N>` is the indicator on if there is continuation for the parameter expression or not;
- `<zzz>` is the reference index/number for the assessment of this parameter;
- The exclamation point ! is used to indicate that the current parameter definition is ended.

PARAMETER NAME

The GES parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Examples of parameter names:

- `G(GAS,C1O2)`: The Gibbs energy of formation of a CO2 molecule in gas.
- `G(FCC,FE:VA)`: The Gibbs energy of formation of fcc Fe with interstitials.
- `L(LIQ,Fe,Cr;0`: The regular solution parameter for Fe and Cr in liquid.
- `L(LIQ,Fe,Cr;1)`: The sub-regular solution parameter.
- `TC(BCC,Fe:Va)`: The Curie temperature of bcc Fe.
- `BMAGN(BCC,Fe:Va)`: The Bohr magneton number parameter of bcc Fe.

The parameter name consists of several parts. The first is a type-identifier and these can be used:

- `G`: Standard energy parameter (Gibbs energy of formation) or for interaction parameters;

- `L`: Excess energy parameter (Gibbs energy of interaction) always used for interaction parameters;
- `TC`: Curie temperature for magnetic ordering;
- `BMAGN` or `BM`: Bohr magneton number for magnetic ordering (or Born function ωPr,Tr for aqueous solute species).
- `VO`: Molar volume at 298.15 K and 1 bar (a numeric value only);
- `VA`: Integrated thermal expansivity; $\int_{298.15}^{T} \alpha\ (T)dT\int_{298.15}^{T} \alpha\ (T)dT$
- `VB`: Bulk modulus at 1 bar;
- `VC`: Isothermal compressibility;
- `VK`: High-pressure fitting parameter.

When necessary quantities as `H` (enthalpy), `S` (entropy), `V` (Volume), `F` (Helmholtz energy), etc., can be calculated from the Gibbs energy.

PHASE NAME

Specifying the `PHASE NAME` in uppercase is recommended; however, if you prefer to write it as a mixture of uppercase and lowercase, it automatically converts all lowercase to uppercase, as the GIBBS module only recognises uppercase phase names. It is important that if a phase bears a legal phase-type (among `G`, `A`, `Y`, `L`, `I`, `F` and `B`) in its phase definition (already by the `PHASE` keyword; such as GAS:G, LIQUID:L,SLAG:L, IONIC-LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name when ENTER_PARAMETER is executed.

CONSTITUENT ARRAY

The constituent array consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents (as the following prompt).

Solution phases with sublattices can have interacting constituents in each sublattice.

INTERACTION PARAMETER

An interaction parameter, which is used to describe the excess term of a quantity, must have two or more constituents that interact with each other on a specified sublattice site of the given phase. It is arbitrary which of these constituents is given as the first constituent and what is given as the interacting constituents. The software always sorts the constituents (in each sublattice) in alphabetical order when the parameter name is written as a prompt (for entering its parameter value) and when the parameter is listed (using the GIBBS commands *LIST_PARAMETER* on page 102 or *LIST_PHASE_DATA (from GIBBS)* on page 103). This is important for all asymmetric interaction parameters where the sign of the interaction parameter must depend on the appearance order.

Use an asterisk* to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L(FCC_L12,AL,NI:*)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the `FCC_L12` solution phase, while it is independent of all constituents on the second sublattice. An interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk * is calculated with the term of [1∑y (specified constituents)], which implies that in an A-B binary system these `L` parameters are identical (but in higher-order systems, these are different):

- `L(phase,A,B)` is multiplied with X(A)*X(B)

- `L(phase,A,*)` is multiplied with X(A)*(1-X(A))
- `L(phase,B,*)` is multiplied with X(B)*(1-X(B))

If you press <Enter> when you are asked for a parameter name or if you have improperly input the entire parameter name, you are asked for each of these items in the name.

ENTER_PARAMETER

For the PARROT Module, this command is the same and is described here.

Also see *About the ENTER_PARAMETER Command* on page 95 for details about each of the options.

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command *AMEND_PARAMETER* on page 44.

Syntax	ENTER_PARAMETER

Prompts	`PARAMETER: <PARAMETER NAME>`
	As explained in *About the ENTER_PARAMETER Command* on page 95, specify a correct and complete `Parameter Name`, which should contain all the necessary parts of the general form:
	`<IDENTIFIER>(<PHASE>,<CONSTITUENT ARRAY>;<DIGIT>)`
	If a parameter name is not acceptable or <Enter>, is pressed, a message displays:
	`*** Error, please re-enter each part separately`
	and you are prompted for input for each required part for a parameter name.

Options	**Description or Information**
`IDENTIFIER`	`IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.
`PHASE NAME`	`PHASE NAME (/ABCD/): <PHASE NAME>` Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.

Syntax	ENTER_PARAMETER
CONSTITUENT	`CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME>` A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated. It is the species name, not the stoichiometric formula required here. If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing <Enter> if the constituent is the same, or specify a new species name.
INTERACTING CONSTITUENT	For phases with several sublattices, the program asks for one constituent in each sublattice. `INTERACTING CONSTITUENT (IN SUBLATTICE  # /XYZ/): <SPECIES NAME>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> to accept it if the constituent is the same, or specify a new species name. To cancel the default value of the interacting constituent type `NONE` or the name of another constituent. This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an <Enter> is enforced.
DEGREE	`DEGREE /#/: <DEGREE>` Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (`L`), Curie temperature (`TC`) and Bohr magneton number (`BMAGN`), as well as for volume-related parameters (`V0`, `VA`, `VB`, `VC` or `VK`). For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index. For a standard `G` parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.
PHASE PARAMETER	After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.

Syntax	ENTER_PARAMETER

	`LOW TEMPERATURE LIMIT /298.15/: <LOWEST TEMPERATURE LIMIT IN K>`
	Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	`FUNCTION: <DEFINITION FOR A FUNCTION>`
	A TP-Function consists of terms in T and P.
	`& <CONTINUATION OF THE DEFINITION FOR THE CURRENT FUNCTION>`
	Continuation of a TP-Function definition.
	`HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K>`
	Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the *lowest limit* is entered as a negative number) for the current TP-Function.
	`ANY MORE RANGES /N/: <Y OR N>`
	Enter `Y` for more function(s) or `N` to end this command.

LIST_ALL_VARIABLES

Create a list of the values and status of all variables in the PARROT workspace on screen or in a text file. After an optimization some statistical information is also written. The correlation matrix is written if that option is chosen.

Also see *SET_OUTPUT_LEVELS* on page 115.

Syntax	LIST_ALL_VARIABLES
Prompt	`OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME>` A list of the current values and status, as well statistical information (if after optimization) and the correlation matrix (optionally), for all variables is written on screen (by pressing <Enter>) or on the list file under a specific file name which can later on be opened and edited by basic text editor.
	Example Output The following is the listed variables for the example TCEX36, after the first optimization when having set all variables available for optimization.

```
== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1  TO V00

VAR.   VALUE                START VALUE         SCALING FACTOR    REL.STAND.DEV
```

Syntax	LIST_ALL_VARIABLES

```
V1      2.03729090E+04    2.03688352E+04    2.03688352E+04
3.41524152E+00

V2     -2.94286372E+01   -2.94286372E+01   -2.94286372E+01
2.37944771E+00

V11    -2.17373936E+04   -2.18095983E+04   -2.18095983E+04    3.97086303E-
02

V12     1.52107184E+01    1.51660547E+01    1.51660547E+01    5.84552327E-
02

V15     2.42082351E+04    2.45139169E+04    2.45139169E+04
5.00914471E+00

V16    -8.38723972E+00   -8.83460472E+00   -8.83460472E+00
1.60961318E+01

V17     3.08916533E+03    3.15802558E+03    3.15802558E+03
9.63738108E+00

V19     2.20292586E+04    2.21385673E+04    2.21385673E+04
4.14274011E+01  V20    -7.04217974E+00   -7.22424882E+00   -7.22424882E+00
1.00561540E+02

NUMBER OF OPTIMIZING VARIABLES :   9

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM   8.00002729E+04 TO   8.00002719E+04

DEGREES OF FREEDOM   45.  REDUCED SUM OF SQUARES   1.77778382E+03
```

LIST_CONDITIONS

In the PARROT module, generate a list of the current values of optimization conditions, as well the current status of listing, either on screen or in a basic text file which can be opened and edited by a text editor.

Syntax	LIST_CONDITIONS
Prompt	`OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME>` Press <Enter> to output to screen or on the list file under a specific file name.

LIST_PARAMETER

This command is for both the GIBBS and PARROT modules.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

```
THE PARAMETER NAME: <IDENTIFIER>(<PHASE>,<CONSTITUENT ARRAY>;<DIGIT>)
```

For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

Syntax	LIST_PARAMETER

Prompts	`PARAMETER: <PARAMETER NAME>`
	Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)
	See *About the ENTER_PARAMETER Command* on page 95 to learn how to define the Parameter Name.
	If a parameter name is not acceptable or <Enter> is pressed, an error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each required part for a parameter name.

	`IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK>` Specify one of these types of legal identifiers.
	`PHASE NAME (/ABCD/): <PHASE NAME>` Specify the phase name.
	`CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME>` Specify the constituent name on the specified sublattice site of the given phase.
	`INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME>` Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	`INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME>` If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.
	`DEGREE /#/: <DEGREE>` Specify a numerical number as the degree for the phase parameter.

LIST_PHASE_DATA (from GIBBS)

All data for a specific phase are written on screen. The thermochemical parameters listed for each phase are always in SI units.

Syntax	LIST_PHASE_DATA
Prompt	`PHASE NAME: <PHASE NAME>` Specify a phase name.

LIST_RESULT

List the result of the current optimization run on screen or in a specified file. The level of detail listed can be prescribed by the command *SET_OUTPUT_LEVELS* on page 115.

The LIST_RESULT command has an option `G` for creation of an experimental data file with two columns, one for the experimental value and the other for the calculated value. It allows plotting a diagram and visualizing the fitting results. The plot is automatically plotted and you can scale it giving commands in the POST module. The option `D` lists all experiments, including those with fulfilled inequalities which are suppressed with the default option `C`.

Syntax	LIST_RESULT
Prompt	`FULL, CONDENSED, DETAILED OR GRAPHIC FORMAT: /C/: <C OR D OR F OR G>`
	Choose a format. • `C` (condensed) is the default. • `D` (detailed) lists all experiments, including those with fulfilled inequalities (not included with the default condensed file). • The `G` (graphical) format creates an experimental data file containing two columns, one with the experimental value and the other with the calculated value. This allows plotting of a diagram where all symbols should be on the diagonal if the fit is perfect. The plot is automatically plotted and you can scale it giving commands in the POST module. • The `F` (full) format is obsolete but retained for backward compatibility. `OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME>` A list of the current optimization results are written on screen (by pressing <Enter>) or on the list file under a specific file name which can later on be opened and edited by basic text editor.
	The output normally consists of these parts: • A title showing the data of the action; • A message on successful optimization with the iteration number in the last optimization;

Syntax	LIST_RESULT
	• A paragraph describing the optimization condition; • A list of the latest set of optimized and fixed variables; • A paragraph describing the optimization quality (some statistical information); • A correlation matrix for all optimizing variables (optionally shown, pre-set by the SET_OUTPUT_LEVELS command); • A list of all parameters (including their symbol names, status and current values or function expressions), and all phase descriptions (including phase name, model names, constituents, and phase's `G/L/TC/BM` expressions) predefined for each phase in the system (optionally shown, pre-set by the SET_OUTPUT_LEVELS command); • A paragraph describing the alternate equilibria (and possible error during optimization); • A detailed list on all the equilibrium points used in the current optimization. If the alternate-mode is used in the optimization, only an error value is shown. For normal-mode calculations, a list is shown for the experimental equilibrium numbers (first column) and corresponding original experimental data (second column, in the form `quantity = value`) which are used in optimization (i.e. non-zero weighted points). Such experimental data are by each point compared by the calculated value (third column) after the last optimization. Also listed are the experimental error (column 4), the difference between the calculated value and original experimental data (column 5), and the contribution to the sum of least square (column 6).

Example Output

The following is the listed result in the example TCEX36 (in the *Console Mode Examples Guide*.), after the first optimization based on the prescribed definitions in the TCEX36a.TCM and TCEX36b.TCM, but having set all variables available for optimization.

```
=====================================================

           OUTPUT FROM P A R R O T.
=====================================================

*** SUCCESSFUL OPTIMIZATION. ***      NUMBER OF ITERATIONS:  10

== OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
```

```
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   1   DMAX =  1.00000000E+02   H =  1.00000000E-04    ACC = (INITIAL SUM
OF SQUARES) *  1.00000000E-03
== OPTIMIZING VARIABLES ==
AVAILABLE VARIABLES ARE V1  TO V00
VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
V1      2.03749463E+04    2.03729090E+04    2.03729090E+04    3.41455863E+00
V2     -2.94286372E+01   -2.94286372E+01   -2.94286372E+01    2.37944774E+00
V11    -2.17395673E+04   -2.17373936E+04   -2.17373936E+04    3.98405298E-02
V12     1.52107184E+01    1.52107184E+01    1.52107184E+01    5.82861832E-02
V15     2.42106560E+04    2.42082351E+04    2.42082351E+04    5.07239609E+00
V16    -8.38723972E+00   -8.38723972E+00   -8.38723972E+00    1.69546796E+01
V17     3.08947424E+03    3.08916533E+03    3.08916533E+03    9.85220694E+00
V19     2.20314615E+04    2.20292586E+04    2.20292586E+04    4.16329629E+01  V20    -
7.04217974E+00   -7.04217974E+00   -7.04217974E+00    1.03161466E+02
NUMBER OF OPTIMIZING VARIABLES :   9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM   8.00002719E+04 TO   8.00002709E+04
DEGREES OF FREEDOM   45.  REDUCED SUM OF SQUARES   1.77778380E+03
Number of alternate equilibria           14
SYMBOL        STATUS   VALUE/FUNCTION
R         80000000  8.3145100E+00
RTLNP     20000000 +R*T*LN(1E-05*P)
V1        48000000  2.0374946E+04
V2        48000000 -2.9428637E+01
V11       48000000 -2.1739567E+04
V12       48000000  1.5210718E+01
V15       48000000  2.4210656E+04
V16       48000000 -8.3872397E+00
V17       48000000  3.0894742E+03
  21 V19       48000000  2.2031462E+04   22 V20       48000000 -7.0421797E+00
LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU                              CONSTITUENTS: A,B
      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
```

```
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T

      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T       L(LIQUID,A,B;1) =
500.00<T< 2000.00: +V13+V14*T

A2B

  2 SUBLATTICES, SITES  2:  1     CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =

             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)

BCC

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU                              CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: 0.0

      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: 0.0

      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T

      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T

FCC

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU                              CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: 408

      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T

      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T

      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T

======  BLOCK NUMBER  1

DEFINED CONSTANTS

    DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

    HTR=HM(LIQUID)-HM(A2B)

Alternate equilibrium calculation                 0.4183

Alternate equilibrium calculation                 0.1932

Alternate equilibrium calculation                 0.1016

Alternate equilibrium calculation                 1.4354E-03

Alternate equilibrium calculation                 2.5063E-02

Alternate equilibrium calculation                 8.3929E-03

Alternate equilibrium calculation                  141.4

Alternate equilibrium calculation                  141.4

Alternate equilibrium calculation                  141.4

Alternate equilibrium calculation                  141.4

Alternate equilibrium calculation                 1.2532E-03

Alternate equilibrium calculation                 5.4781E-04
```

```
Alternate equilibrium calculation                    1.5404E-03
Alternate equilibrium calculation                    1.2702E-03
ACR(B)=9.4E-1               0.9397      2.85E-02 -2.7745E-04 -9.7472E-03
ACR(B)=8.4E-1               0.8395      2.82E-02 -4.9038E-04 -1.7396E-02
ACR(B)=7.4E-1               0.7407      2.81E-02  7.3804E-04  2.6305E-02
ACR(B)=6.4E-1               0.6424      2.81E-02  2.3935E-03  8.5272E-02
ACR(B)=5.4E-1               0.5434      2.82E-02  3.4449E-03  0.1220
ACR(B)=4.4E-1               0.4428      2.85E-02  2.8265E-03  9.9024E-02
ACR(B)=3.4E-1               0.3394      2.90E-02 -5.8174E-04 -2.0040E-02
ACR(B)=2.3E-1               0.2320      2.97E-02  2.0260E-03  6.8208E-02
ACR(B)=1.2E-1               0.1194      3.06E-02 -6.4192E-04 -2.0981E-02
HMR(LIQUID)=-1964           -1957.      5.00E+02   7.439      1.4878E-02
HMR(LIQUID)=-3500           -3478.      5.00E+02   21.67      4.3338E-02
HMR(LIQUID)=-4588           -4565.      5.00E+02   22.69      4.5382E-02
HMR(LIQUID)=-5239           -5217.      5.00E+02   21.50      4.3008E-02
HMR(LIQUID)=-5454           -5435.      5.00E+02   19.11      3.8216E-02
HMR(LIQUID)=-5233           -5217.      5.00E+02   15.50      3.1008E-02
HMR(LIQUID)=-4575           -4565.      5.00E+02   9.691      1.9382E-02
HMR(LIQUID)=-3481           -3478.      5.00E+02   2.669      5.3385E-03   118  HMR
(LIQUID)=-1950          -1957.      5.00E+02  -6.561     -1.3122E-02
```

LIST_STORE_FILE

Syntax	LIST_STORE_FILE
	Displays the name of the store file and its full path.

LIST_SYMBOL_IN_GES

Lists TP-function(s) for the entered model parameters for phases in the system on screen. In many cases, the optimizing variables are parts of the TP-functions which in turn are entered in model parameters for various phases in the GIBBS workspace.

This command is a way to find out how the functions depend on the optimizing variables. In the PARROT module the list is only shown on screen, not written to any file (which the LIST_SYMBOL command in the GIBBS module does).

Syntax	LIST_SYMBOL_IN_GES
Prompt	`NAME: <SYMBOL NAME>` Specify a symbol name. Only those symbols that match this name are listed. Or press <Enter> for a list of all available symbols entered in the system.

OPTIMIZE_VARIABLES

Perform variable optimization. All system-definition data needed for the optimization is read from the current work file (*.PAR). The result of the optimization is automatically stored in the current work file.

Syntax	OPTIMIZE_VARIABLES
Prompt	`NUMBER OF ITERATION /N/: <INTEGRAL NUMBER OF ITERATION>` Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT module tries this number of different sets of values of the optimizing variables unless it has converged earlier, or has given up earlier.
	It initially takes a small step in each variable to find the steepest slope. You can give zero iteration to calculate the error in all selected experiments, and then use *LIST_RESULT* on page 104to check how good (bad) the current fit is.

READ_PARROT_WORKSPACES

Read the previous PARROT/GIBBS/POLY3 workspaces back to replace the current PARROT/GIBBS/POLY3 workspaces. It is useful if late changes made through various PARROT/GIBBS/POLY commands are not satisfactory.

Syntax	READ_PARROT_WORKSPACES
	The previous PARROT/GIBBS/POLY3 workspaces are always associated with the latest action to either open a work file by *SET_STORE_FILE* on page 116, or to create a work file by *CREATE_NEW_STORE_FILE* on page 94 (either interactively in the PARROT module or through a *MACRO_FILE_OPEN* on page 5 of an *SETUP.TCM file), or to update the work file by *SAVE_PARROT_WORKSPACES* on page 111.
	Unlike the READ commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to read a previously opened/created/updated PARROT/GIBBS/POLY3 workspaces, for the reason described above.

Syntax	READ_PARROT_WORKSPACES
	You cannot use this command if there is no work file opened or created already.

RECOVER_VARIABLES

Syntax	RECOVER_VARIABLES
	The values of all variables are set back to the start values.

REINITIATE

This command should not be used unless you want to destroy the current PARROT workspace. However, this PARROT command does not reinitiate the GIBBS/POLY3 workspaces.

Syntax	REINITIATE
	The workspace used by the PARROT program is reinitiated. All output and optimizing conditions are given their default values. All variables are set fixed with their value equal to zero.

RESCALE_VARIABLES

Syntax	RESCALE_VARIABLES
	The current values of all the parameters are copied to their start values and the scaling factors for further optimization. Thus it should be done now and again, in particular if you think the optimization results are improved after the previous run(s), or if any variable changes more than a factor of 10.

SAVE_PARROT_WORKSPACES

Syntax	SAVE_PARROT_WORKSPACE
	If the latest changes made through various PARROT/GIBBS/POLY commands are as required, use this command to save the current workspace (i.e. data area) used by the PARROT program (also including the current GIBBS and POLY3 workspaces), onto the present work *.PAR file which has already been opened by *SET_STORE_FILE* on page 116 or been created by *CREATE_NEW_STORE_FILE* on page 94 (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file). The PARROT/GIBBS/POLY3 workspaces are updated after each PARROT/GIBBS/POLY command. This means the current PARROT/GIBBS/POLY3 workspaces are always updated onto the latest work *.PAR file that is associated with the latest SET_STORE_FILE or CREATE_NEW_STORE_FILE command.
	Unlike the SAVE commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to save the current PARROT/GIBBS/POLY3 workspaces, for the reason described above. You cannot use this command if there is no work *.PAR file opened or created already.

SET_ALTERNATE_MODE

Turn the alternate mode on or off. The alternate mode is described in *PARROT Commands* on page 86. It should be used only to optimize start values of the model parameters in the beginning of the assessment.

With the ALTERNATE mode is possible to include functions to be evaluated together with an alternate calculation and to select ALTERNATE mode for each experimental equilibrium.

Syntax	SET_ALTERNATE_MODE
Prompt	`ON /Y/: <Y OR N>` The default `Y` turns on the alternate mode.

SET_EXTERNAL_PARAMETER

Optimize model parameters of the so-called external models, which may not be as fully-implemented/integrated parts inside the GIBBS system and thus are independently defined within user-specified/written source codes. This command makes links between the PARROT optimizing variables and external model parameters.

In order to be able to build the specified external model and to use this SET_EXTERNAL_PARAMETER command, it requires you to first write codes for a preferred external model (as it is not within the standard GIBBS system of the Thermo-Calc software) and then provide it to the consultancy team (consult@thermocalc.se) of Thermo-Calc Software Company in Stockholm for the purpose of including the external model in a separate DLL that is interactively connected to the Thermo-Calc software. Such a special service can/should only be provided under the restrictive condition that a specific Consultancy Project Contract is bilaterally agreed and signed in advance between users and Thermo-Calc Software.

Syntax	SET_EXTERNAL_PARAMETER
Prompt	`EXTERNAL NAME: <PARAMETER NAME IN THE EXTERNAL MODEL>` Correctly specify the parameter name defined within a specified/written external model.

	`AS OPTIMIZING VARIABLE NUMBER: <N>`
	Give the number of the PARROT optimizing variable, which should have a unique link to the specified parameter name of the external model.
	For example, @@ Link PARROT variables to CAM parameters:
	`SET-EXTER-PAR GT(SLAG_A,O-2,SI+4,CA+2) 1`
	`SET-EXTER-PAR ET(SLAG_A,O-2,SI+4,CA+2) 2`
	`SET-EXTER-PAR EXT(SLAG_A,O-2,SI+4,CA+2) 3`

SET_FIX_VARIABLE

Prescribe a fixed value to a variable. The variable is considered as a constant at the optimization, usually after successful optimization runs for some specific variables (for some of the phases in the system). Such fixed variables can also be set back for further optimization run by using *SET_OPTIMIZING_VARIABLE* on page 114.

Syntax	SET_FIX_VARIABLE
Prompts	`VARIABLE NUMBER: <VARIABLE NUMBER(S)>` Specify the number of the variable. It is possible to give a range by giving two numbers with a hyphen in between (no spaces allowed), e.g. `1`. The parameters within the limits are set fixed to their current values (no question of values).
	`START VALUE /XXXX.XXXXX/: <A VALUE TO BE FIXED>` Specify a numerical value to be fixed for the selected variable (only when one variable number is specified at the previous prompt). The current value for the selected variable is

Syntax	SET_FIX_VARIABLE
	shown as default. If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values are used as fixed values.

SET_OPTIMIZING_CONDITION

Specify the conditions for the optimization. The default values are chosen automatically by the PARROT program, and in most cases these should not be changed.

The optimization stops when the sum of errors decreases by this value, even though it might be possible to increase it further with a new OPTIMIZE command.

Syntax	SET_OPTIMIZING_CONDITION
	`RELATIVE STANDARD DEVIATION FOR EXPERIMENTS? /N/: <Y OR N>` Choose whether the standard deviation of the experimental determinations are absolute values (`N`) or if these are used as relative weighting factors (`Y`). The estimated standard deviations of the optimized variables might be different for the two cases.
Prompt	`MIN SAVE ON FILE? /Y/: <Y OR N>` Specify whether the program should minimize the transfer of data to and from the current work file during the optimization: If Y, it speeds up the optimization. After optimization use the *SAVE_PARROT_WORKSPACES* on page 111 command to update the progress onto the current work file. If minimum saving on file is not specified (`N`), the workspaces are stored on the current work file after every iteration in the optimization procedure.
	`ERROR FOR VARIABLE BOUNDS: /1/: <RETURN >` This feature has not been implemented yet. Press <Enter>.
	`RELATIVE STEP FOR CALCULATION OF DERIVATIVES: /1E-04/: <XXX>` In the calculation of the correlation matrix for equilibria with inaccuracy in the independent state variables, some numerical derivatives might have to be calculated. Specify the relative step (`xxx`) for the calculation of these derivatives.
	`MAXFUN (VA05AD): /100/: <N>` The maximum number of iterations in the optimization. The same value set by the OPTIMIZE command.

Syntax	SET_OPTIMIZING_CONDITION
	`DMAX (VA05AD): /100/: <N>` An estimate of the maximum distance between the start and the final values of the variables. A smaller value makes the program vary the parameters with smaller factors.
	`H (VA05AD): /1E-04/: <XXX>` The step used in the scaled variables for calculating numerical derivatives during the optimization.
	`ACC/(INITIAL SUM OF SQUARES) (VA05AD): /.001/: <XXX>` The break condition for the optimization. The accepted value is the difference between the true minimum and the calculated one.

SET_OPTIMIZING_VARIABLE

Specify which variable value should be estimated at the optimization. Such a variable can have a value of zero or another start value, or is fixed by *SET_FIX_VARIABLE* on page 112 prior to the previous optimization run.

For a good reference prior to this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as pre-entered in the *SETUP.TCM file or interactively entered in the GIBBS module) are obtained by using *LIST_ALL_VARIABLES* on page 101.

Syntax	SET_OPTIMIZING_VARIABLE
Prompts	`VARIABLE NUMBER: <VARIABLE NUMBER(S)>` Specify the number(s) for the variable(s) to be set. Any non-zero parameter within the range is allowed to be optimized. A parameter with a current value equal to zero must be specified explicitly here in order to be optimized. Specify a range by giving two numbers connected by a hyphen (no space allowed!), e.g. `2-8`. Under this circumstance, no question of start values are asked.
	`START VALUE /XXXX.XXXXX/: <A GUESS VALUE>` Specify a start guess of the optimum value (only when one variable number is specified at the previous prompt). The current numerical value for the selected variable is shown as default. This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria. If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values (as start values) are not changed.

SET_OUTPUT_LEVELS

Choose the type of information the PARROT module gives during the optimization procedure and when listing results.

Syntax	SET_OUTPUT_LEVELS
Prompts	`LIST INCREMENT /1/: <INCREMENT IN ITERATION NUMBER>` Specify the increment in iteration number for which information is listed on screen during the optimization. By giving a larger number it shortens the list.
	`LIST SUM OF SQUARES: /Y/: <Y OR N>` Choose whether the sum of squares is listed on screen during the optimization procedure.
	`LIST SCALED VARIABLES: /Y/: <Y OR N>` Choose whether the scaled variable values are listed on the terminal during the optimization procedure.
	`LIST WEIGHTENED RESIDUALS: /N/: <N OR Y>` Choose whether the weighted residuals are listed on the terminal during the optimization procedure.
	`LIST ALL PARAMETERS: /N/: <N OR Y>` Choose whether all parameters in the models are listed in *LIST_RESULT* on page 104.
	`LIST CORRELATION MATRIX: /N/: <N OR Y>` Choose whether the correlation matrix of the variables are listed with the commands LIST_RESULT and *LIST_ALL_VARIABLES* on page 101.

SET_SCALED_VARIABLE

This command is similar to *SET_OPTIMIZING_VARIABLE* on the previous page in that it specifies start values for optimizing variables. The difference being it is functional for only one optimizing variable at one time. It also prescribes a minimum and maximum value for the variable. During the optimization runs, the variable value is limited within this min-max range.

Such a variable may have a value of zero or another start value, or may be fixed by *SET_FIX_VARIABLE* on page 112 prior to the previous optimization run. For a good reference prior to using this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as entered in the *SETUP.TCM file or interactively entered in the GIBBS module) is obtained by using *LIST_ALL_VARIABLES* on page 101.

Syntax	SET_SCALED_VARIABLE
Prompts	`VARIABLE NUMBER: <VARIABLE NUMBER(S)>` Specify the number for an optimizing variable to be set. Any non-zero parameter is allowed to be optimized, and a parameter with a current value equal to zero must be specified explicitly here in order to be optimized.
	`START VALUE /XXXX.XXXXX/: <A GUESS VALUE>` Specify a start guess of the optimum value. The current numerical value for the selected variable is shown as default. This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria.
	`MIN VALUE /XXXX.XXXXX/: <A GUESS VALUE>` Specify a minimum guess of the optimum value. It should be smaller than, at least equal to, the current start value for the selected variable.
	`MAX VALUE /XXXX.XXXXX/: <A GUESS VALUE>` Specify a maximum guess of the optimum value. It should be larger than, at least equal to, the current start value for the selected variable.

SET_STORE_FILE

Specify a store file (work file) to be used for compilation and optimization. The *.PAR work file must be created (*CREATE_NEW_STORE_FILE* on page 94) as a store file. The GIBBS, POLY and PARROT workspaces are read from the specified store file (with a default extension of PAR).

Syntax	SET_STORE_FILE
Prompt	Enter an `*.PAR file name` in the **File name** field and specify the working directory in the **Look in** field. Normally the default file-type in the **Files of type** field is the correct one for the PARROT workspace format (i.e. *.PAR file). Click **Open** or **Cancel** as applicable.

POLY_3 Commands

In this section:

ADD_INITIAL_EQUILIBRIUM

Add initial equilibrium points from which a phase diagram is calculated (through the *MAP* on page 158 command).

Syntax	ADD_INITIAL_EQUILBRIUM
Prompt	`DIRECTION /DEFAULT/: <DIRECTION CODE>` `direction code (s)` `1` or `2` for positive direction of axis 1 or 2, respectively; `-1` or `-2` for negative direction of axis 1 or 2, respectively; `Default` for all directions. The direction is important when the initial equilibrium point is in a single-phase region or when the phase diagram is an isopleth (tie-lines not in the plane of calculation). In such cases, the program searches for a line in the diagram (i.e. a line where the amount of a phase is zero, imply that if it starts to become stable on one side of the line and disappear on the other side) in the given direction.

Normally, this command is not needed to calculate a property diagram (with the *STEP_WITH_OPTIONS* on page 172 → `NORMAL` command-sequence). In many cases, the ADD_INITIAL_EQUILBRIUM command is not required for MAP commands either, as the mapping procedure starts from the current equilibrium state already calculated. In order to calculate a simple phase diagram, set the equilibrium conditions and the mapping axis variables, and then give a MAP command. But if a phase diagram has disconnected lines, the ADD_INITIAL_EQUILBRIUM command may still be needed to add two or more initial equilibria so that the MAP calculation starts from such initial equilibria at the specified directions to find all phase boundary lines.

This command becomes unnecessary in most cases, as the MAP routines that by default use the Global Minimization Technique handles all the initial equilibrium points in a robust and automatic way. Therefore, you do not need to have a good guess of the starting point and to add any initial equilibrium point prior to the calculations of various types of phase diagrams. However, if preferred, use this command to add any initial equilibrium points in certain directions, the POLY module uses the specified starting point(s) and corresponding user-added initial equilibrium point(s) for a mapping calculation; in such a case, the automatic procedure in the rewritten MAP routines are not enforced while the Global Minimization Technique can still be applied. Similar situations occur when a specific database, in which there are some definitions of initial-equilibrium adding direction(s) for accessed binary and/or ternary subsystems in its ACCESSED_SYSTEM section, is used in the BINARY or TERNARY module for calculating a binary or ternary phase diagram.

The ADD_INITIAL_EQUILBRIUM command with the default direction scans along the axis variables and generates start points each time the scanning procedure crosses a phase boundary. In addition, it generates four start points, scanning cross the middle of each axis, if there is any solubility line that does not reach the axes. At the MAP command, a search for lines in the diagram is made along each direction of the axis variables in the diagram. In this way, it should guarantee that all possible phase boundary lines in a phase diagram are found. Of course, it may take a little longer time to execute than using the minimum number of start points, as some lines may be calculated more than once. But the POLY module remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria by appending a > after the direction at the ADD command. For example:

```
Direction /default/: 2>
```

```
Direction /default/: -2>
```

This generates one start point for each set of phase change in the positive direction of the axis 2 (or negative direction of the axis 2); this ensures finding all possible phase boundary lines (not just the first one) along such an axis direction.

This is particularly useful when you have a phase diagram with several lines with no intersection. It is thus possible to calculate e.g. an isopleth for a much more limited composition range. It is also useful for calculating CVD diagrams and Pourbaix diagrams.

All the initial equilibrium points generated by the ADD_INITIAL_EQUILBRIUM command (previously and presently; saved in the current POLY workspace) can be easily listed out on screen with *LIST_INITIAL_EQUILIBRIA* on page 157. A certain initial equilibrium point (including its conditions and equilibrium results) can be loaded into the current equilibrium, if needed, with *LOAD_INITIAL_EQUILIBRIUM* on page 158. Any specific or all of the initial equilibrium points can be deleted from current POLY workspace, if desired, with *DELETE_INITIAL_EQUILIBRIUM* on page 151.

ADVANCED_OPTIONS Descriptions

Also see *ADVANCED_OPTIONS* on page 125 for information about the command.

These ADVANCED_OPTIONS can be set:

EQUILIBRIUM_CALCUL

Designed to decide how to perform the Ordinary POLY Minimization (i.e. the traditional Gibbs Energy Minimization) in the POLY module. By default, the Global Minimization Technique for various single point equilibrium calculations and for stepping or mapping calculations is used. You can use the advanced option *GLOBAL_MINIMIZATION* on page 236 to permanently turn off (for all sequential calculations throughout the current TCC run) the Global Minimization Technique and consequently use only the Ordinary POLY Minimization, and additionally adjust the ways to proceed the normal minimization (mainly in terms of how to control the steps in reaching Gibbs energy minima in an equilibrium state). When enforcing the Global Minimization Technique in the equilibrium calculations, you can further adjust the manners for assigning grid-points and for handling new possible compositional set(s) for solution phases during stepping/mapping; since the Global Minimization Technique also uses the normal POLY optimization routine for some calculations, it is also possible to change the ways on how to control the steps in reach Gibbs energy minima in an equilibrium state, in order to improve convergence.

GLOBAL_MINIMIZATION

Designed to decide how to perform the so-called Global Minimization in the POLY module. By default, the POLY module uses the Global Minimization Technique for various single-point equilibrium calculations and for stepping or mapping calculations. You can use this to permanently (for all sequential calculations throughout the current TCC run) turn off the Global Minimization Technique and consequently use only the Ordinary POLY Minimization, and additionally adjust the ways to proceed the normal minimization (mainly in terms of how to control the steps in reaching Gibbs energy minima in an equilibrium state). When enforcing the Global Minimization Technique in the equilibrium calculations, you can adjust the manners for assigning grid-points and for handling new possible compositional set(s) for solution phases during stepping/mapping; since the Global Minimization Technique also uses the normal POLY optimization routine for some calculations, it is also possible to change the ways on how to control the steps in reach Gibbs energy minima in an equilibrium state, in order to improve convergence.

LIST_PHASE_ADDITION

The values set as additional contributions (given by PHASE_ADDITION) to Gibbs energy *G*m (J/mol formula unit) to all the phases (stoichiometric or solution) are listed at the current calculated equilibrium.

MAJOR_CONSTITUENTS

Use this to set the major constituent(s) of a composition sets in a miscibility gap of a solution phase. Normally, the major constituents are specified when a new composition set is created by the NEW_COMPOSITION_SET option; but for the first composition set, this option may be needed before using NEW_COMPOSITION_SET.

NEW_COMPOSITION_SET

A solution phase that can exist with two (or more) different compositions simultaneously must have two (or more) composition sets in its phase descriptions. Normally the database creates as many composition sets as is necessary but use this command to add or delete more composition sets. A complex solution phase in a defined multicomponent system can have up to 9 different composition sets for the purpose of appropriately handling its possible miscibility gap(s) under various temperature-pressure-composition conditions.

This option is unnecessary if the Global Minimization Technique is in use, as it can automatically detect all possible miscibility gap(s) for complex solution phases (normal or disordered/ordered phases) and then automatically add required composition sets for such phases in the defined system.

This option can automatically create composition sets also for disordered phase when it is executed for the ordered phase.

If you have your own data file, this option must be used to indicate that a solution phase can have a miscibility gap (or may exhibit some complex phase separations as to more than two composition sets), unless that the possibly-additional composition set(s) for the solution phase must have already been added inside the TDB file (through a TYPE_DEFINITION command to amend composition-set) or been manipulated through the GIBBS module (using the AMEND_PHASE_DESCRIPTION COMPOSITION_SET command-sequence). This option asks for default major constituents for the new sets and it is important that this is set correctly, otherwise the test for miscibility gaps may fail.

OUTPUT_FILE_FOR_SHOW

The name of a text file is asked for and all the results output from the command SHOW_VALUE is written to this file.

PARAEQUILIBRIUM

This calculates a paraequilibrium between two specific phases in an alloy system with one or more interstitial component(s) as fast diffusion species. Under the paraequilibrium state, two partially-equilibrated phases have the same chemical potential (but different contents) for one or more interstitial components (such as C, N, O, S, etc., as individual or combined)], along varied temperature or along a composition variable (of the matrix or one substitutional component) which has already set as the stepping variable with *SET_AXIS_VARIABLE* on page 164.

To ensure a successful point calculation of paraequilibrium state between two specific phases in a defined alloy system, it is important that you first have made a single-point equilibrium calculation with an initial overall composition in the current system before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable. The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true for cases where there are more than one interstitial components to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviours as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.

Note the following:

Always check if the chosen phases A and B have the exactly same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).

Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and staring bulk composition for the system.

Always set the status of the chosen interstitial components as SPECIAL using the POLY command: *CHANGE_STATUS* on page 135 `Component <interstitial component> = SPECIAL`. By doing this, you get a clear picture of u-fractions of various substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

PHASE_ADDITION

Sometimes it is interesting to add a constant contribution to the Gibbs energy of a phase (stoichiometric or solution). This can be done in the Database Module (DATA) or Gibbs Energy Module (GIBBS), for a stoichiometric phase, or for a pure end-member in a solution phase. However, if the addition is related to the equilibrium state, for example, strain energies or surface energies, interfacial energies or deformation energies, it may be more convenient to have this quantity related to the equilibrium state rather than the thermodynamic data.

Give a value of an addition to the Gibbs energy of a phase. The value should always be constant (implying that the addition is not a function of phase composition or temperature-pressure conditions in the equilibrium state) and always be given in the unit of J/mol formula unit of the phase.

PRESENT_PHASE

The phase specified must be stable at all equilibria calculated during a *MAP* on page 158 command. It is a way to limit the calculations of the monovariant lines in a ternary system to those in the liquidus surface. Normally such a calculation would have two compositional axes and a temperature axis and all monovariant lines, also those between 3 solids, would be mapped. If the liquid is set as PRESENT, only those with the liquid is mapped.

SHOW_FOR_T=

Display various thermodynamic properties (state variables, derived/partial variables or entered symbols) of the currently calculated (stable/meta-stable) equilibrium state but under a different temperature condition. This is useful for knowing, for example, a volume-related property of a frozen (stable/meta-stable) equilibrium state at a certain temperature, where the equilibrated phase assemblage and all the phase compositions are not adjusted while only the temperature condition is changed.

Use this option carefully. You must have successfully calculated a real equilibrium state under one temperature condition (normally the temperature for the last heat treatment). This can then be used to obtain the value(s) of any specified state variable(s) or derived/partial variable(s) or defined symbol(s) for thermodynamic properties of the entire system, of components, or of phases for the currently-defined system (being in a frozen state) under another temperature (normally at room temperature). No real equilibrium is re-calculated through this option, and thus the phase amounts and compositions in the system are the same as at the last real equilibrium calculation.

STABILITY_CHECK

In some composition ranges of a multicomponent system, it often happens that an unstable solution phase region locates inside a miscibility gap, and the stability limit (the *spinodal curve* or *spinodal*) may be not easy to find. A system inside a spinodal is thermodynamically unstable with respect to compositional fluctuations, and the system may experience the *spinodal decomposition* (i.e. decomposing to a mixture of regions with the two stable compositions, one on each side of the miscibility gap).

This option makes it possible to automatically check internal stability of both stable and unstable phases in all subsequent single-point equilibrium and MAP/STEP calculations. It can find out if any phase is subject to spinodal decomposition during the subsequent calculations. If there is an unstable phase located inside a miscibility gap in a calculation, it gives a warning so that you suspend the unstable phase, or use FORCED automatic start values for phase constituents (i.e. *SET_ALL_START_VALUES* on page 162 → `FORCE` command-sequence), or create other composition sets; you can also ignore the warning message if you know that the unstable phase is not formed in the current calculations.

STEP_AND_MAP

This is the default and is used to determine how to perform Global Minimization test and how to handle initial equilibrium points.

T-ZERO_TEMPERATURE

This calculates the temperature when two specific phases have the same Gibbs energy, i.e. the so-called T0 temperature. You must calculate an equilibrium state at an estimated temperature before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium state in which either one or both of the target phases is stable.

TOGGLE_ALTERNATE_MODE

Toggle the ALTERNATE mode for experimental equilibrium calculation between DEFAULT, ALWAYS and

NEVER, during data-assessments using the PARROT optimization.

ADVANCED_OPTIONS

Also see *ADVANCED_OPTIONS Descriptions* on page 120.

Syntax	ADVANCED_OPTIONS
Prompt	`WHICH OPTION? /STEP_AND_MAP/:  <OPTION>`
Options	**Description and Information**
`NONE`	Take away any set advanced option in all subsequent single-point equilibrium and MAP/STEP calculations. If there is any convergence problem in finding a stable solution, at any stage of an advanced option calculation conducted by an ADVANCED_OPTIONS command-sequence, these messages display: `Convergence problems, increasing smallest site-fraction from 1.00E-30   to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS` The smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command *SET_NUMERICAL_LIMITS* on page 237 to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

`STEP_AND_MAP`
(the default)
	Settings for MAP and STEP:
	`GLOBAL TEST INTERVAL /0/: <INTEGER NUMBER>`
	Settings for MAP:
	`AUTOMATICALLY ADD INITIAL EQUILIBRIA /Y/: <Y OR N>`
	`NUMBER OF MESH ALONG AN AXIS /3/: <INTEGER NUMBER>`
	`USE INSIDE MESHING POINTS /N/: <Y OR N>`
	`GLOBAL TEST INTERVAL /0/: <INTEGER NUMBER>`
	The integer number determines how often the Global Minimization should be used during STEP_WITH_OPTIONS and MAP calculations. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during STEP calculations, and only at node points during MAP calculations. Any other positive integer number, n, suggests it performs a Global Minimization test at every *n*-th step during STEP and MAP calculations. Of course, the Global Minimization test is always carried out at a phase change or a node

Syntax	ADVANCED_OPTIONS

	point. The Thermo-Calc software is installed with 0 (zero) as the default value, but such a configuration for the default value can be changed by using SET_TC_OPTIONS in the SYS module.
	`AUTOMATICALLY ADD INITIAL EQUILIBRIA /Y/: <Y OR N>`
	When *ADD_INITIAL_EQUILIBRIUM* on page 119 is not used before MAP, a mesh of initial equilibrium points are added before the mapping itself takes place. This mesh is only available when two (2) axes are already defined. The default on start-up may be changed by SET_TC_OPTIONS in the SYS monitor.
	`NUMBER OF MESH ALONG AN AXIS /3/: <INTEGER NUMBER>`
	An integer for how many intervals of initial equilibrium points to be added along an edge in the diagram. For example, if set to 2 (two), initial equilibrium points are added at the beginning, centre, and end of each axis-variable forming 2 intervals.
	`USE INSIDE MESHING POINTS /N/: <Y OR N>`
	If `N` the INITIAL_EQUILIBRIUM mesh consists of initial equilibrium points added only along the edge/border of the diagram defined by the axis-variables. If `Y`, the initial equilibrium points added are also added inside edge.

`EQUILIBRIUM_CALCUL`	The following prompts affect the ways how the POLY optimization does the Ordinary POLY Minimization to reach the minimum of an equilibrium state.
	Settings for the minimization of an equilibria:
	`FORCE POSITIVE DEFINITE PHASE HESSIAN /Y/: <Y OR N>`
	`CONTROL STEPSIZE DURING MINIMIZATION /Y/:  <Y OR N>`
	`FORCE POSITIVE DEFINITE PHASE HESSIAN /Y/: <Y OR N>`
	Choose `Y` or `N` to determine how to reach the minimum of an equilibrium state in a normal POLY optimization procedure. This is related to the special quantity, the phase stability function QF (phase), for all kinds of phases in an equilibrium state [A phase stability function for a phase is negative when the phase composition is inside a spinodal, and positive everywhere else].
	If the composition of a solution phase is inside its spinodal, the enforcement of positive definite eigenvalues of a Hessian matrix (i.e. by answering Y) makes the step be taken towards the minima rather than the local maxima. Furthermore, if an eigenvalue (for a phase) of the Hessian matrix is near 0.0, the step-size is large and the answering `Y` sets a lower limit to this eigenvalue, and reduces the step-size and improves the convergence. The POLY command-sequence SHOW_VALUE QF(phase) shows the size of the lowest eigenvalue of a phase in an equilibrium state.

Syntax	ADVANCED_OPTIONS
	By answering `Y` it might help the Ordinary POLY Minimization to converge, if there is such a problem, especially if QF(phase)=0 for phases. By answering `N` the Ordinary POLY Minimization routine is applied. For each phase in a defined system, the molar Gibbs energy of the phase is a function of the temperature-pressure condition and its composition: $G_m(X) = G_m(T,P;y_1,y_2,...,y_n)$ Compute a Hessian matrix as which describes the curvature of the Gibbs energy curve of this phase at the defined composition X: $\partial^2 G_m / \partial y_i \partial y_j$ Diagonalise this matrix and call the Eigenvalues as e1,e2,...,en . The QF(phase) quantity for this phase is the lowest of these eigenvalues divided by the same values for a corresponding ideal (stoichiometric) phase: $QF(ph) = \min(\{e_1,e_2,...,e_n\}) / \min(\{se_1,se_2,...,se_n\})$ Here, se1,se2,...,sen are the eigenvalues for the ideal phase. Therefore, for an ideal (stoichiometric) phase, the QF(phase) should always be 1.0. `CONTROL STEPSIZE DURING MINIMIZATION /Y/: <Y OR N>` Choose `Y` or `N` to determine whether to introduce a control of step-size while reaching the minimum of an equilibrium state in a normal POLY optimization procedure. By answering `Y` it might help the POLY optimization to converge, especially if when some site fractions are less than 1E-4.

GLOBAL_ MINIMIZATION	The following prompts affect how the Global Minimization is done. Settings for global minimization:
	`USE GLOBAL MINIMIZATION AS MUCH AS POSSIBLE /Y/: <Y OR N>`
	`USE GLOBAL MINIMIZATION FOR TEST ONLY? /N/: <Y OR N>`
	`MAXIMUM NUMBER OF GRIDPOINTS PER PHASE /2000/: <INTEGER NUMBER>`
	`USE GLOBAL MINIMIZATION AS MUCH AS POSSIBLE /Y/: <Y OR N>`
	Choose `Y` or `N` to decide if using the Global Minimization Technique from start of calculation or not. The default value on start-up may be changed by SET_TC_ OPTIONS in the SYS module.
	If `Y` the calculation is done when possible (depending on the condition settings), and a Global Minimization test is always performed when an equilibrium is

Syntax	ADVANCED_OPTIONS

	reached. This costs more computer time but the calculations are more accurate.
	If `N` the calculation is not used to reach the equilibrium state. `Use global minimization for test only?` determines if the Global Minimization test is made against the calculated equilibrium states obtained by the Ordinary POLY Minimization calculation.
	`USE GLOBAL MINIMIZATION FOR TEST ONLY? /N/: <Y OR N>`
	If `Y` a calculated equilibrium state obtained by the Ordinary POLY Minimization calculation is tested against the Global Minimization Technique after it is reached; and if found it as unstable, there is an error message.
	If `N` the Global Minimization Technique is never tested for or done for all sequential calculations throughout the current TCC run. This implies that Global Minimization Technique is permanently turned off, and that consequently only the Ordinary POLY Minimization routine is used.
	`MAXIMUM NUMBER OF GRIDPOINTS PER PHASE /2000/: <INTEGER NUMBER>`
	Specify the maximum number of grid points that are computed for each of the phases in the currently defined system, during the calculations enforced by the global minimization. More grid points give a higher robustness and take more computation time. The total number of computed grid points in all phases is limited to `2E6`.

`IGNORE_COMPOSI_ SET_ORDER`	`IGNORE COMPOSITION SET ORDER /N/`

`NEW_ COMPOSITION_SET`	The following prompts are to specify the additional composition set(s) to handle possible miscibility gap(s) of a certain solution phase:
	`PHASE WITH MISCIBILITY GAP: <NAME OF A PHASE>`
	Specify the name of the phase with miscibility gap.
	`NEW HIGHEST COMPOSITION SET NUMBER /2/: <#>`
	The default value is usually one higher than the current value. Each phase has initially one composition set. If a lower value is given, composition sets are deleted. You cannot take away the first composition set.
	A message displays to show that you need to specify the composition for the composition set # (2,3,…).
	`MAJOR CONSTITUENT(S) FOR SUBLATTICE 1: /XX/: <YY>`
	The major constituents (`YY`) in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps

Syntax	ADVANCED_OPTIONS
	should have different major constituents for each composition set. This prompt is repeated for each sublattice in the phase, sometimes even for all sublattices in the first composition set if such major constituents have not been specified.

`MAJOR_ CONSTITUENT`	The following prompts are to specify the major constituent(s) on each of the sublattice sites for a composition set of a certain solution phase:
	`PHASE NAME: <NAME OF A PHASE>`
	Specify the name of the solution phase with a new set of major constituents.
	`COMPOSITION SET NUMBER /1/: <#>`
	The default value for the composition set number (#) is usually /1/ as the other composition sets are given major constituents when creating them. Each phase has initially one composition set.
	`MAJOR CONSTITUENT(S) FOR SUBLATTICE 1: /XX/: <YY>`
	The major constituents (`YY`) on each sublattice of a solution phase can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.
	This question is repeated for each sublattice in the phase.

`PHASE_ADDITION`	The following prompts are to specify the additional energy term (always being a constant) of a given phase.
	`PHASE NAME: <NAME OF A PHASE>`
	Specify the name of the (stoichiometric or solution) phase with the addition.
	`ADDITION TO G PER MOLE FORMULA UNIT: <XXXXX>`
	The value (`xxxxx`) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy or whatsoever.
	It is not composition-, temperature- or pressure-dependent.

`LIST_PHASE_ ADDITION`	No additional prompt.
`PRESENT_PHASE`	Specify the name of the present phase a the name of the phase that should be present at all calculated equilibria:

Syntax	ADVANCED_OPTIONS
	`PRESENT PHASE:` `PHASE NAME: <NAME OF A PHASE>`

`T-ZERO TEMPERATURE`	`NAME OF FIRST PHASE:  <PHASE A>`
	`NAME OF SECOND PHASE: <PHASE B>`
	The names of phases A and B must be given, for which the T0 temperature (where the Gibbs energies are equal) is to be calculated.
	If the T0 temperature between the two specified phases is successfully calculated, a message displays, e.g.
	`THE T0 TEMPERATURE IS 840.82 K. NOTE: LIST-EQUILIBRIUM IS NOT RELEVANT`
	The first message shows the calculated T0 temperature between the two specified phases.
	The second message indicates that after this option calculation with LIST_ EQUILIBRIUM is irrelevant and does not list the equilibrium for the system at the T0-temperature.

`PARAEQUILIBRIUM`	`NAME OF FIRST PHASE:  <PHASE A>`
	`NAME OF SECOND PHASE: <PHASE B>`
	The names of the two target phases A and B, between which the paraequilibrium state is to be calculated, must be entered subsequently or on the same (first) line at once then separated by an empty space, e.g. `FCC#1 BCC` or `FCC#2 M23C6`.
	You need to understand what you are dealing with in terms of calculating a paraequilibrium state between the two specified phases.
	Specifically, there are four distinguished cases to understand: (1) both chosen phases must have similar interstitial/vacancy sublattices where the fast-diffusion interstitial component(s) occupy; (2) the choice on the target phase pair must be reasonable for the defined system and specified initial overall composition; (3) both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or (4) it is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.
	`FAST DIFFUSING COMPONENT: /C/: <INTERSTITIAL COMPONENT(S)>`
	`FAST DIFFUSING COMPONENT: /NONE/: <INTERSTITIAL COMPONENT(S)>`
	The name(s) of the fast-diffusing component(s) (C as the default single

Syntax	ADVANCED_OPTIONS

	component) must be given at the above prompts subsequently or at the same (first) prompt. It is possible to specify more than one interstitial component as fast diffusion species.
	Note the following:
	Such specified interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: these must be located on the interstitial/vacancy sublattices in both chosen phases;
	If there is only one fast-diffusing component which is carbon, press the <Enter> key to accept the default input at the first prompt; if the single fast-diffusing component is another element (e.g. N), type its name at the first prompt;
	If there are two or more fast-diffusing components (e.g. `C` and `N`), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as `C N`);
	To finish the input of fast-diffusing elements, accept NONE at a repeated prompt, i.e. by pressing <Enter> key to start the paraequilibrium point calculation;
	If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus cancelled entirely.
	If the paraequilibrium state between the two specified phases is successfully calculated, the messages displays e.g.
	`NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02  N = 4.1548129E-03`
	`NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04  N = 2.3781027E-04`
	`All other compositions the same in both phases`
	`Note: LIST-EQUILIBRIUM is not relevant`
	The first and second lines list the phase amounts expressed in mole-percent [NP (phase)] and the contents of the interstitial components C and N in a specific phase expressed in the so-called u-fractions [u-f(phase,C) and u-f(phase,N)], for the phase A (in this case as FCC) and phase B (in this case as BCC), respectively. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) in both the target phase A and target phase B are the same at the current paraequilibrium state, while these are not shown on screen. The last line indicates that after this advanced-option calculation the LIST_EQUILIBRIUM command is irrelevant and does not list the paraequilibrium state for the system at the current condition.

Syntax	ADVANCED_OPTIONS

	However, if the single-point calculation of the paraequilibrium state between the two specified phases has failed, these messages display:
	`*** ERROR     4 IN NS01AD`
	`*** NUMERICAL ERROR`
	This implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component(s). Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.

`STABILITY_CHECK`	`STABILITY CHECK ON? /Y/: <Y OR N>`
	The default is `Y` to switch on the automatic stability check during all subsequent single-point equilibrium and MAP/STEP calculations. By answering `N`, there is no stability check in various calculations.
	`CHECK ALSO FOR UNSTABLE PHASES? /Y/: <Y OR N>`
	If the automatic stability-check option is switched on choose to also check the stability for unstable phases. The default is `Y` and if an unstable phase is found to be located in a miscibility gas during a subsequent single-point equilibrium or MAP/STEP calculation, a warning message informs you to selectively make adjustments in the calculation settings [e.g. suspending the unstable phase, or using FORCED automatic start values for phase constituents by the S_A_S_V F command-sequence, or creating other composition sets, etc.]. By answering `N` the stability check is enforced only to stable phases in the system.

`TOGGLE_ ALTERNATE_MODE`	`SET ALTERNATE TOGGLE TO DEFAULT, ALWAYS, OR NEVER?`
	`SET GLOBAL TOGGLE TO DEFAULT, ALWAYS, OR NEVER?`
	`DEFAULT` means that the experiment points are calculated according to the Alternate Technique depending on the SET_ALTERNATE command.
	`ALWAYS` means the experiment points are always calculated according to the Alternate Technique even if the Alternate Mode is switched off in the PARROT module.
	`NEVER` means the experiment points are calculated as normal equilibria even if you SET_ALTERNATE in the PARROT module.

`SHOW_FOR_T=`	`TEMPERATURE (K) /298.15/: <TEMPERATURE_IN_K>` Specify the new temperature condition (in K) under which the values of some specific state variable(s) or derived/partial variable(s) or defined symbol(s) for

Syntax	ADVANCED_OPTIONS
	various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system (being in a *frozen* state) is shown on screen. `STATE VARIABLE OR SYMBOL /VM/: <STATE VARIABLE OR SYMBOL NAME(S)>` Specify the name(s) of the desired state variable(s) or derived/partial variable(s) or defined symbol(s) for various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system. More than one state variable or symbol of interest can be simultaneously specified on the same line. For example, you can choose to show the values of VM or GM (i.e. molar volume or molar Gibbs energy of the entire system), or of VM(*) or HM(*).T (i.e. molar volumes or isobaric heat capacity of all phases), or of ACR(*), DGM(*) and LNACR (*,FCC) [i.e. activities of all system components, driving forces for all phases, and activities (in logarithm) of all system components in the FCC solution phase], under the new temperature condition (being in a frozen state).
`OUTPUT FILE FOR SHOW`	A window opens with a default name for the file `tc_show.dat`. Choose a location to save the file and click Open.

AMEND_STORED_EQUILIBRIA

This command gives information about the calculated blocks (and phase regions included in blocks) after the STEP or MAP calculation(s). It allows you to list all or part of the calculation results, to suspend all or parts of the calculation results that are redundant or where metastable equilibria are calculated, and to restore all or parts of the calculation results (if having been suspended by another AMEND_STORED_EQUILIBRIA command).

The workspace for storing equilibria may overflow during stepping or mapping, and is then written to a file as blocks. Each block usually contains one or more ranges of equilibrium regions.

Use one these options:

- `L` to list the calculated equilibria (all or a specified block)
- `S` to suspend everything (all blocks and their regions)
- `Q` to suspend each set of equilibria individually (specified blocks and/or regions)
- R to restore everything (all blocks and their regions)

Syntax	AMEND_STORED_EQUILIBRIA
Prompts	`NAME: <NAME OF A DEFINED TABLE>` List (`L`) the calculated equilibria, suspend everything (`S`) or suspend each set of equilibria individually (`Q`), or restore everything (`R`).
	`BLOCK /*/: <BLOCK NUMBER>` Specify a block number in the option `L`, `S`, `Q` or `R`. Or include all the blocks in the amending option, by accepting the wildcard * (press <Enter>). For `L`, a block (if a block number is specified) or all the blocks (if the wildcard * is accepted/used), with the regions and the equilibrium details, that are calculated during stepping or mapping is listed on screen or in a textual file. For `Q`, each ranger in a block (if a block number is specified) or in all blocks (if the wildcard * is accepted/used) then choose:

	`S(USPEND) K(EEP) /K/: <S OR K>`
	For `S` or `R`, if a block is specified, you are asked what region in the block should be suspended or restored. However, if the wildcard * is accepted/used, you are asked the following:
	`REALLY SUSPEND ALL /N/: <Y OR N>`
	`REALLY RESTORE ALL /N/: <Y OR N>`
	If the answer is `N`, the program asks for which block(s) and which region(s) in a certain block to execute the `S` or `R` action.
	`REALLY SUSPEND ALL /N/: <Y OR N>`
	`Y` suspends everything.
	`REALLY RESTORE ALL /N/: <Y OR N>`
	`Y` restore everything.

	`RANGE: <RANGE(S) OF REGION>` Specify one or more ranges to be suspended (the `S` option) or restored (the `R` option). The wildcard * suspends or restores all ranges in the specified block. In order to know the ranges the `LIST` option must first be used.
	`S(USPEND) K(EEP) /K/: <S OR K>` The Query suspend option (`Q`) asks for each region in a certain block if it should be suspended or kept. Suspended regions are not included on sequentially generated plots.
	`OUTPUT FILE: /SCREEN/: <FILE NAME>`

Syntax	AMEND_STORED_EQUILIBRIA
	This prompt is only for listing (the `L` option), and after it the command is terminated. The file name must be given here; or accept the default `SCREEN` (terminal) by pressing <Enter>. A list of stored equilibria as various blocks (with all their ranges) are shown out on screen or the file.

CHANGE_STATUS

In the POLY module, set the status for components, species and phases in the defined system for all the sequential calculations (single-point, stepping and mapping) in equilibrium or local/partial equilibrium state. Each component, species and phase has a status. The default status is `ENTERED`.

The most important use is to calculate metastable equilibria and metastable phase diagrams by setting some phases (that would otherwise be stable) to the SUSPENDED or DORMANT phase-status. Another important applications is to calculate paraequilibria by setting some components to the SPECIAL component-status.

For a component and for a species, the status can be one of the following:

- `ENTERED` - the component(s) or species are included in the calculation. This is the default status.
- `SUSPENDED` - the component(s) or species are not considered in the calculation.
- `SPECIAL` means - specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).

Only component(s) can have the status SPECIAL, which implies that these are not included in summations for mole or mass fractions.

For example, for the *u-fractions* or other normalized fractions, when one or more of the components are excluded from the summation, you must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status SPECIAL. This is assigned by the CHANGE_STATUS command.

Syntax	CHANGE_STATUS
Prompts	`FOR PHASES, SPECIES OR COMPONENTS? /PHASES/: <KEYWORD>` `Keyword` = phase or species or components
	`PHASE NAME(S): <NAME(S) OF THE PHASE(S)>` For `phase` as the keyword, the names of the phases that have their status changed must be given (all on one line). A comma or space must be used as separator. The status to be

Syntax	CHANGE_STATUS
	assigned to the phases can also be given on the same line if preceded with an equal sign =. An asterisk, *, can be used to denote all phases. The special notations `*S`, i.e. a wildcard * directly followed by an `S`, sign, means all suspended phases. In the same way, `*D` means all dormant phases, and `*E` means all entered phases.
	`NAME(S): <NAME(S) OF THE SPECIE(S) OR COMPONENT(S)>` For `species` or `component` as the keyword, the names of the species or components that have their status changed must be given (all on one line). A comma or space must be used as separator. Similarly to the case of `phase` as the keyword, the status to be assigned to the species or components can also be given on the same line if preceded with an equal sign =. An asterisk, *, can be used to denote all species or components. The special notations `*S`, i.e. a wildcard * directly followed by an `S`, sign, means all suspended species or components. In the same way, `*E` means all entered species or components.
	`STATUS /ENTERED/: <NEW STATUS>` The `new` status to be assigned must be given. For species, the values `ENTERED` or `SUSPENDED` can be used. For components, the status `ENTERED`, `SUSPENDED` or `SPECIAL` can be given. SPECIAL means that this component is excluded from sums for mole fractions and mass fractions, which is useful when calculating the *ufractions* or other normalized fractions of system components. For phases, the status `ENTERED`, `SUSPENDED`, `DORMANT` or `FIXED` can be given. DORMANT means the same as suspended but the driving force is calculated. FIXED means that it is a condition that the phase is stable at a certain amount. For example, for the ufractions, when one or more of the components are excluded from the summation, you must specify which component should be excluded from the calculation of the mole fraction. This component must have the status SPECIAL. This is assigned by the CHANGE_STATUS command: `Change_Status comp C=special`.
	`START VALUE, NUMBER OF MOLES /0/: <INITIAL AMOUNT>` For ENTERED phases, an `initial amount` of the phase can be given. Normally, 0 is given if the phase is not likely to be stable, and 0.5 or 1 or any positive number if the

Syntax	CHANGE_STATUS
	phase could be stable, but such an initial amount is only used as the rough starting estimation in the equilibrium calculations.

	`NUMBER OF MOLES /0/: <EQUILIBRIUM AMOUNT>`
	For FIXED phases, the `equilibrium amount` of the phase [always using an initial estimation being the `NPF(phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase] must be given. If the equilibrium amount is zero, then the phase is at its stability limit.
	Special attentions should be paid when specifying a FIXED phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below:
	The phase amount variables, NP(phase), BP(phase) and VP(phase), as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, use the CHANGE_STATUS command to set a relevant condition, e.g. `CHANGE_STATUS phase <phase>=fix <amount>` where the fixed <amount> is roughly the same as the F-suffixed quantity `NPF(phase)`.
	The `NPF(phase)` quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other `F`-suffixed state variables [e.g. GF(phase), HF(phase) and DGF(phase)] cannot be directly applied in any POLY command, implying that it cannot be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, you should use a properly-entered symbol (function or variable), for example: `NPFabc = NP (abc)/NA` or `NPFabc = NPM(abc)/NA*N`. N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy). For example, the SIGMA, FCC, BCC and LIQUID phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modelled by certain models, and their NA values must be evaluated in different ways, as described below:
	`LIQUID (C,Cr,CrO3/2,Fe,FeO,FEO3/2,N,Ni,NiO)1` ➔`NA = 1`
	`FCC_A1 (Cr,Fe,Ni)1(Va,C,N,O)1` ➔`NA = 1`
	`BCC_A2 (Cr,Fe,Ni)1(Va,C,N,O)3` ➔`NA = 1`
	`SIGMA (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18` ➔`NA = 30`
	If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase is modelled by the Two-Sublattice Ionic Liquid Model, i.e.:
	`IONIC_LIQ  (Cr+3,Fe+2,Ni+2)p(VA,C,N,O-2,FEO3/2)q,7`
	then the evaluation of its NA value becomes even more complicated:
	`NA = p + q*yC2 + q*yN2 + q*yO2□2 + q*yFeO2 3/ 2`

Syntax	CHANGE_STATUS
	where the stoichiometric coefficients *p* and *q* are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by a multiple sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases. There is no strange thing when using a zero value [i.e. `0`] in a FIXED phase-status, since it means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e. it starts becoming stable on one side of a corresponding phase-boundary line or unstable on the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states. However, when a non-zero value [it must always be positive; e.g. 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific FIXED-status phase in a calculated equilibrium state any longer; instead, the <equilibrium amount> value is the NPF(phase) value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations. Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase is predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e. N=1). When a phase is described by a solution model in which two or more sublattices are considered and these sublattice sites may also have different stoichiometric coefficients [meaning that the mixture phase could have more than one atom in formula [NA>1; see some examples above], the unity value should not be used when setting the FIXED status for the phase; instead, you should use an appropriate value that ranges from 0 to a NPF (phase) value that equals to or is smaller than 1/NA (if the total system size N=1) or 1/NA*N (if N differs from unity). For this reason, if a multicomponent system bears an IONIC_LIQUID phase that is described by the Two-Sublattice Ionic Liquid Model (or any other multiple-sublattice ionic solution phases), it is difficult to use a proper `NPF(ION_LIQ)` value in setting its FIXED phase-status, because that should be less than (or equal to) the complex value of $N/[p + q*^{y}C2 + q*y_{N}2 + q^{*}y_{O}22 + q^{*}y_{FeO}2\ 3/\ 2\ ]$.

Examples

For example, to obtain the metallic fraction in a system with carbon as an interstitial component, you can set the component status for carbon as `SPECIAL`:

```
Change_status comp C=special
```

The `SUSPENDED` status for components and species does not always work as expected.

For a phase, it may have one of these statues:

- `ENTERED` - the phase(s) are included in the equilibrium calculations and these are stable if that minimizes the total Gibbs energy in the defined system. This is the default status for all phases already retrieved from the chosen database(s). An ENTERED phase-status is always associated with an initially-estimated amount [in mole number; normally, as 0 if the phase is not likely to be stable, and as 0.5 or 1 or any positive number if the phase could be stable] but it is only used as the rough starting value in the equilibrium calculations.

- `SUSPENDED` - the phase(s) are not considered in the equilibrium calculations.

- `DORMANT` - the phase(s) are not considered in the equilibrium calculations but their driving forces for precipitation are calculated.

- `FIXED` - it is an equilibrium condition that the status-fixed phase must be stable, and be in equilibrium at a specified amount [always using an initial estimation being the `NPF (phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase]. See more descriptions at the end of this command.

COMPUTE_EQUILIBRIUM

The full equilibrium state is calculated for the given set of conditions. The Global Minimization Technique is by default enforced in this command (C_E), while it can be disabled temporarily (for the current single-point equilibrium calculation) if using C_E – or C_E * command-combination, or permanently (for all the sub sequential single-point calculations or stepping/mapping calculations within the current TCC run) if having decisively switched it off by a user (or possibly in some special modules) through changing the minimization option using the *ADVANCED_OPTIONS* on page 125 → `MINIMIZATION_OPTION` command-sequence.

Syntax	COMPUTE_EQUILIBRIUM
Prompt	The C_E command can be used, in order to enforce the ordinary POLY minimization routines in an equilibrium calculation; this is because of that the ordinary C_E command is now associated with the Global Minimization Technique, and only after the Global Minimization If technique is permanently switched off the C_E command makes no difference from the C_E – command-combination. Only certain types of equilibrium conditions [e.g. `T`, `P`, `N`, `N(<component>)`, `X(<component>)`, `B`, `B(<component>)`, and `W(<component>)`] are fully supported in the Global Minimization mode (called *Direct Global Minimization*); and when other types of equilibrium conditions are used, after the initial POLY, a Global Minimization test and corrections are performed until the lowest minimum is found (called *Indirect Global Minimization*). If there is any problem with convergence, you may try the C_E * command-combination. The character * enforces the command to use an advanced technique to obtain a complex equilibrium. However, after a successful C_E *calculation, you may repeat the C_E command and can check the status of phases, species or components (with *LIST_STATUS* on page 157 → CPS command-sequence) and equilibrium conditions (with *LIST_CONDITIONS* on page 155) and list out the calculation results (with *LIST_EQUILIBRIUM* on page 156), because such actions may tell you how to further modify various settings for your current calculation. This command-combination is not that useful anymore, because the Global Minimization Technique that is always associated with the C_E command is even more powerful and more precise in finding the most-stable equilibrium state in a complex heterogeneous interaction system; therefore, the C_E * command-combination is functional and can be used only after the Global Minimization mode has already been disabled temporarily or permanently. Some phases that are not stable in the current equilibrium state may not have their most favourable composition after this command, and thus their driving forces may not be correct. You can force the program to correctly calculate the driving forces of metastable phases, by giving repeated C_E commands until the number of iterations (that is shown on screen after this command) is reduced to 2. Also see the POLY command *SET_NUMERICAL_LIMITS* on page 237 which can set the approximate driving force for metastable phases option on or off in all the subsequent POLY calculations within the current TCC run. If an equilibrium state for the defined system is not found, an error message is given.

Syntax	COMPUTE_EQUILIBRIUM
	You can try repeating this command a few times, or change some of settings for the numerical limits, for starting variables and starting values, for starting constitutions of certain phases and for reference states of certain components, or to verify some of the defined conditions.

COMPUTE_TRANSITION

This command is a combination of the CHANGE_STATUS, SET_CONDITION and COMPUTE_EQUILIBRIUM commands. It allows a direct calculation when a new phase may form by varying one of the already-set conditions. It can be used only after at least one equilibrium is calculated successfully; otherwise, you are informed on the necessity of first making an equilibrium calculation to find out the stable phases under the current conditions.

When this command is used, the program calls the command *CHANGE_STATUS* on page 59 to temporarily change the phase status of a specified phase as FIXED at the *zero* amount, and at the same time to temporarily release one of the existing equilibrium conditions (which is chosen by you). The program calculates a new equilibrium in which that specific phase is stable but its equilibrium amount in the system is zero. The released condition is then assigned with a calculated value that ensures the calculated equilibrium. Afterwards, the program automatically changes the phase status of that specific phase back to ENTERED, and resets the temporarily released condition as one of the conditions and assigns it with the value that is calculated to ensure the zero-amount formation of that specific phase.

This command is useful to find melting temperature, boiling temperature, or solubility limits, and generally when you want to set the most optimal conditions for calculating an equilibrium where a specific phase becomes stable. It can also be used when you want to know exactly how far away the defined conditions are from the value that can ensure a zero-amount of a specific phase in the system when other conditions remain the same.

After a successful COMPUTE_TRANSITION calculation, you can issue a *COMPUTE_EQUILIBRIUM* on page 139 calculation to assure the calculated transitional equilibrium is a really stable one, and can also use *LIST_EQUILIBRIUM* on page 156 to see the details of transitional equilibrium state.

Syntax	COMPUTE_TRANSITION

Prompts

`PHASE TO FORM: <PHASE NAME>`

A new `phase name`, e.g. `BCC` that is expected to form, is specified here. This changes the status of this new phase to be `FIXED` as `0` amount, and the program shows the information such as:

```
You must remove one of the these conditions
P=100000, T=800, N=1, X(FE)=.5    DEGREE OF FREEDOM 0
```

If the key word `ANY` is used when prompted for `Phase to form` (instead of a specific phase name), it is possible to find out any new phase to be formed, in a given varying direction sign and at an estimated change of the released condition: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but it is only estimated value, so any value within its reasonable scale would be enough). Such calculations can be repeated if required. This feature is useful to find out all possible phase transformations along a certain released condition.

`GIVE THE STATE VARIABLE TO BE REMOVED /T/: <ONE CONDITION>`

`One condition` must be removed, in order to calculate the transition equilibrium where the specified (or any) new phase to be formed at a calculated value of this released variable.

Therefore, the message may display (after a successful calculation) if, for example, `X (Fe)` is entered:

```
To form BCC the condition is set to X(FE)=.48605791769
```

This calculated value is assigned as the parameter of that removed condition, in this case, the `X(FE)` variable. If the LIST_CONDITIONS command is typed this message displays:

```
P=100000, T=800, N=1, X(FE)=4.86057918E-1
DEGREES OF FREEDOM 0
```

If the key word `ANY` (instead of a specific phase) is given as the phase name when it is prompted for Phase to form, the line is prompted for a given varying direction sign and an estimated change of the released condition before the calculation of transition equilibrium:

`ESTIMATED CHANGE (WITH SIGN) /1/: <+/-#>`

A given varying direction sign and an estimated change of the released condition, in this case as `X(FE)`, must be given here: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but

Syntax	COMPUTE_TRANSITION
	it is only estimated value, so any value within its reasonable scale would be enough). For example, if a combination of -0.02 is input, this message may display (after a successful calculation):

```
To form BCC_A2#1 the condition is set to X(FE)=.493708756187
```

This calculated value is then assigned as the parameter of that removed condition, in this case, the `X(FE)` variable. The message is shown if the LIST_CONDITIONS command is typed:

```
P=100000, T=800, N=1, X(FE)=4.93708756E-1

DEGREES OF FREEDOM 0
```

CREATE_NEW_EQUILIBRIUM

During data-assessments using the PARROT/ED_EXP modules, you can, in the POLY module, create several equilibria with different sets of conditions and phases (but normally with the same set of components). By default, there is one equilibrium. To keep the set of conditions and phase for this equilibrium, create another one using this command, and use another set of conditions for that. Two equilibria may be useful to calculate easily the enthalpy difference between two states. In the PARROT module, the experimental information is stored as a sequence of equilibria.

Syntax	CREATE_NEW_EQUILIBRIUM
Prompts	`EQUILIBRIUM NUMBER /2/: <A NEW EQUILIBRIUM NUMBER>` Each equilibrium in the POLY3 workspace is identified by a unique integer number. Such an equilibrium number can be recalled with *SELECT_EQUILIBRIUM* on page 162.
	`INITIATION CODE /2/:` When an equilibrium is created, you can choose to `ENTER` all components and phases (initiation code 2), `ENTER` the components only (initiation code 1) or `SUSPEND` everything (initiation code 0). No other values are legal. The entered components and phases can later be changed with *CHANGE_STATUS* on page 59.

DEFINE_COMPONENTS

Change the set of components. By default, the elements are used as components. The set of components can be important because some conditions are set using components, for example, the amounts, activities or chemical potentials.

For example, in the system Fe-Si-O, you can define FEO, FE2O3 and SIO2 as components, thus replacing the default FE, SI and O.

This implies a command *REINITIATE_MODULE* on page 161 and it should be given as the first command in the POLY module.

Syntax	DEFINE_COMPONENTS
Prompt	`GIVE ALL NEW COMPONENTS /EXISTING COMPONENTS/: <NEW COMPONENTS>` The `new components` must be specified all on one line. These replace the existing component definitions. The number of components cannot be changed with this command. Use *CHANGE_STATUS* on page 59 instead.
	To keep some existing components, it is recommended that you also enter these on the line. Otherwise, the added new components may not be defined correctly. This is especially important if some components are built out of several elements. The new components do not have to be present as species.

DEFINE_DIAGRAM

This allows automatic calculation and plotting of a diagram with a single command. It is the same as the DEFINE_MATERIAL command up to when the first equilibrium is calculated. The alloy OPTION feature is also available in this command to specify alloying compositions for a special alloy predefined by the OPTION keyword in a selected database (e.g. the TCNI Ni-based Superalloys Database).

Use this command to calculate all types of phase diagrams after specifying all composition value and an initial temperature (if temperature is used as an axis). However, for binary and ternary diagrams, the special BIN and TERN modules may be preferred.

It then lists all the independent variables for the defined system (i.e. temperature and the components) and asks for a variable as the X-axis. You must also specify a maximum and minimum for the X-axis. The second axis (Y-axis) can be another composition (or the temperature if that is not on the X-axis) from the independent variable list. The program then calculates and plots a *phase diagram*, as there are two independent quantities on the axes.

Alternatively, select a dependent quantity as the Y-axis variable from the second list on screen (e.g. the amount of all phases, composition of a specific phase, or fractions of a component in all phases), and the program calculates and plots how this quantity depends on the condition on the X-axis. This is a *property diagram*.

This command ends up within the POST module monitor. You can refine the calculated phase diagram or property diagram.

Moreover, many more property diagrams with axes other than compositions can also be plotted (after the calculation), using *SET_AXIS_VARIABLE* on page 164 in the sequent POST monitor.

Syntax	DEFINE_DIAGRAM

Prompts	These prompts are given:
	`SAME ELEMENTS AS BEFORE /Y/? <Y OR N>`
	`MOLE PERCENT OF <ELEMENT> /##/: <VALUE>`
	or
	`MASS PERCENT OF <ELEMENT> /##/: <VALUE>`
	`DATABASE /ABCDE/: <DATABASE NAME>`
	`MAJOR ELEMENT OR ALLOY: <ELEMENT NAME>`
	`COMPOSITION IN MASS (WEIGHT) PERCENT? /Y/: <Y OR N>`
	`1ST ALLOYING ELEMENT: <ELEMENT NAME>`
	`MASS (WEIGHT) PERCENT: <AMOUNT OF THE ABOVE SPECIFIED ELEMENT>`
	`2ND ALLOYING ELEMENT: <ELEMENT NAME>`
	`NEXT ALLOYING ELEMENT: <ELEMENT NAME>`
	`MASS (WEIGHT) PERCENT: <AMOUNT OF THE ABOVE SPECIFIED ELEMENT>`
	`TEMPERATURE (C) /1000/: <TEMPERATURE OF INTEREST IN OC>`
	`REJECT PHASE(S) /NONE/: <LIST OF PHASE(S) TO BE REJECTED>`
	`RESTORE PHASE(S) /NONE/: <LIST OF PHASE(S) TO BE RESTORED>`
	`OK? /Y/: <Y OR N>`
	`SHOULD ANY PHASE HAVE A MISCIBILITY GAP CHECK? /N/: <Y OR N>`
	`PHASE WITH MISCIBILITY GAP: <PHASE NAME>`
	`MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AA/: <CONSTITUENT(S)>`
	`PHASE WITH MISCIBILITY GAP: <PHASE NAME>`
	The first equilibrium is calculated, as with *DEFINE_MATERIAL* on page 147. Then a list of all independent conditions suitable to be chosen as X/Y-axis variables is given by the program.

	`QUIT? /Y/: <Y OR N>` This question is asked only when the axis variables are already defined, or if the command DEFINE_DIAGRAM is used. It then offers an opportunity to quit (`Y`) the calculation or to continue (`N`) the calculation but by defining other axes.
	`GIVE THE NUMBER OF THE CONDITION TO VARY /1/: <A CONDITION INDEX>`

Syntax	DEFINE_DIAGRAM
	Select one of the independent conditions by giving its index on the condition list as the X-axis variable.
	`MINIMUM VALUE /XXX/: <MINIMUM VALUE FOR X-AXIS>` Specify the minimum value of the chosen X-axis variable. A default value is shown automatically by the program; press <Enter> to accept it or input another value.
	`MAXIMUM VALUE /YYY/: <MAXIMUM VALUE FOR X-AXIS>` Specify the maximum value of the chosen X-axis variable. A default value is shown automatically by the program; press <Enter> to accept it or input another value. Then another list with some dependent quantities is given by the program, which can be selected as the Y-axis variable.
	`GIVE THE NUMBER OF THE QUANTITY ON THE SECOND AXIS /#/: <##>` Select one of the independent conditions or dependent quantities as the Y-axis variable, by giving its corresponding index given on the condition lists. It must be different from the X-axis variable already selected. If selecting one of dependent quantities (by giving the corresponding number from the second list) as the Y-axis, then a property diagram is to be automatically calculated (through a normal stepping procedure) and generated. For `composition of a phase` the phase name is asked for further specification subsequently. If selecting any of the other independent variables (conditions) on the first list as the Y-axis, then a phase diagram is automatically calculated (through a mapping procedure) and plotted.
	`NAME OF PHASE: /ABC/: <PHASE NAME>` This is prompted only in case of that the `composition of a phase` is selected as the Y-axis variable. The phase name for which the composition varied along with X-axis variable should be specified.
	`MULTIPLE START POINTS? /Y/: <Y OR N>` This question is to confirm whether or not to let the program to automatically generate and use multiple start points for mapping the defined phase diagram.
	`SAVE FILE /RESULT/: <FILE NAME>` The file name where the calculations are stored (saved as a *.POLY3 file) should be specified; the default file name is `RESULT.POLY3` (Windows) or `RESULT.poly3` (Linux).

DEFINE_MATERIAL

Read data for a system from a database in the POLY module. It is convenient to use for alloys when there is a major component and the amount of the other elements is known in mass (weight) fraction. The command reads the system from the specified database, sets the composition and temperature (and pressure equal to 1 bar) and calculates the equilibrium state before the prompting for a new command. You can list the results with *LIST_EQUILIBRIUM* on page 156 or set a new composition or set axis for a STEP or MAP command.

You cannot append data from different databases in this way. Use this command with data from a USER database.

Syntax	DEFINE_MATERIAL
Prompts	`SAME ELEMENTS AS BEFORE /Y/? <Y OR N>` This question is asked only if some data is already read from the database, or if the command DEFINE_MATERIAL or DEFINE_DIAGRAM is used. It then offers a convenient way to change the composition and temperature with one command. This command only works properly in cases where the composition of the material system is already defined as in the mole-percent or mass-percent unit.

	`MOLE PERCENT OF <ELEMENT> /##/: <VALUE>`
	or
	`MASS PERCENT OF <ELEMENT> /##/: <VALUE>`
	If you have decided to use the same materials system (available in the current POLY3 workspace) by accepting the default answer (`Y`) to the previous prompt `Same elements as before /Y/?`, one of the alternative prompts display for each of the components in the defined system, depending on how the composition is defined (either in mole-percent, or in mass-percent).
	Prompts are repeated until all the defined components are completed. Then, the program prompts to specify the temperature condition.

	`DATABASE /ABCDE/: <DATABASE NAME>` The database with the description for the material must be given, or press <Enter> if using the current database. It is possible to give a USER database.
	`MAJOR ELEMENT OR ALLOY: <ELEMENT NAME>` The material must have a major element, usually the element which is present in the largest amount. The fraction of this element is not set but is the rest.

Syntax	DEFINE_MATERIAL
	In some databases there are the alloys predefined. An alloy has a default major element and have limits of the amounts of the alloying elements. If you stay within these limits the calculation gives reasonable results.
	`COMPOSITION IN MASS (WEIGHT) PERCENT? /Y/: <Y OR N>` The default is that input is taken as mass percent, but it is possible to change to mole percent by answering `N`. Composition should be given in PERCENT not FRACTION, as it is required for the `W` and `X` state variables in the *SET_CONDITION* on page 165 command.
	`1ST ALLOYING ELEMENT: <ELEMENT NAME>` The first alloying element must be given. All alloying elements are asked for in a sequence. These can be given in any order. You must know if you are present as assessed systems in the database. There is no error or warning messages if data are missing. Check the documentation of the database selected. If an alloy is selected, a list of legal alloying elements and their maximum percent is listed on-line.
	`MASS (WEIGHT) PERCENT: <AMOUNT OF THE ABOVE SPECIFIED ELEMENT>` The amount of the alloying element in mass (weight) percent. Using the DEFINE_ MATERIAL command you cannot use the normal flexibility of Thermo-Calc for conditions, but all must be given in mass percent. However, you can afterwards change the conditions using the SET_CONDITION command.
	`2ND ALLOYING ELEMENT: <ELEMENT NAME>` The second alloying element must be given. If only one, press <Enter>. If an element name is given then the program asks for its mass fraction.
	`MASS (WEIGHT) PERCENT: <AMOUNT OF THE ABOVE SPECIFIED ELEMENT>` The amount of the above specified alloying element in mass (weight) percent.
	`NEXT ALLOYING ELEMENT: <ELEMENT NAME>` Continue giving elements and mass (weight) fractions until all elements specified. When all alloying elements and their compositions (as in the above prompt) are specified, press <Enter> as answer to this question to finish the materials definition.
	`TEMPERATURE (C) /1000/: <TEMPERATURE OF INTEREST IN OC>`

Syntax	DEFINE_MATERIAL
	POLY makes the first calculation after retrieving the data for this temperature. By pressing <Enter> to accept the default temperature. The value should be given in Celsius (oC). The pressure is set to 1 bar.
	`REJECT PHASE(S) /NONE/: <LIST OF PHASE(S) TO BE REJECTED>` This is a question generated by the database allowing you to select the phases. Normally, all phases should be included when you press <Enter>. If a phase is to be rejected, the name of the phase must be supplied. Several phase names can be specified in one line. It is possible to reject all phase by giving an asterisk *. If the number of phases to be included is much smaller than the total number of phases, it may be convenient to first reject all phases and then restore those that should be included. The question is repeated until you press <Enter> after rejecting all unwanted phases or an asterisk *.
	`RESTORE PHASE(S) /NONE/: <LIST OF PHASE(S) TO BE RESTORED>` You can restore phases that are accidentally or deliberately rejected. It may also be possible to restore some hidden phases. If phases are to be restored the name of the phases must be supplied. Several phase names can be specified in one line. It is possible to restore all phase by giving an asterisk *. The question is repeated until you press <Enter> after restoring all desired phases.
	`OK? /Y/: <Y OR N>` All phases to be selected from the database are listed and the selection confirmed. If there are any errors or you want to amend the selection, answer `N` and you are returned to the question about rejecting phase(s). If the selection is confirmed by answering `Y` the software retrieves all thermodynamic data and available references from the chosen database.
	`SHOULD ANY PHASE HAVE A MISCIBILITY GAP CHECK? /N/: <Y OR N>` The database usually creates two or more composition sets for phases that can have miscibility gaps. However, for some phases this is not done automatically, for example the miscibility gap in the bcc phase in Fe-Cr is usually ignored. But if it is important to include a Cr-rich bcc phase, specify this here. It costs some computation time and may make the subsequent MAP or STEP more difficult to converge. If you do not want to have any phase with a miscibility gap in the calculation, press <Enter>. Then, the DEFINE_MATERIAL command starts calculating the equilibrium, and is terminated.
	To set such a phase with miscibility gaps in the calculation, answer `Y`. Then the software

Syntax	DEFINE_MATERIAL
	asks questions about the phase names and their constitutions, such as: `PHASE WITH MISCIBILITY GAP: <PHASE NAME>` You must supply the phase name, which has a miscibility gap under the specified system and conditions.
	`MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AA/: <CONSTITUENT(S)>` The software shows a default constituent in the sublattice `#(1,2,3,…)`, according to the existing phase definition in the chosen database. You can specify one or more major constituents for the sublattice # in the phase. This question is repeated until all sublattices are specified.
	`PHASE WITH MISCIBILITY GAP: <PHASE NAME>` You can supply another phase name with a miscibility gap under the specified system and conditions, and answer the questions concerning the major constituent(s) in associated sublattice(s). By pressing <Enter>, the command starts calculating the equilibrium, and then terminates.
	It is also possible to use this command to select an alloy from a specific database (e.g. the TCNI Ni-based Superalloys Database). Such alloys are predefined by the OPTION keyword inside the database, and have their default major elements and composition limits of their alloy elements. Such alloys available in the selected database (at the prompt `Database /ABCDE/` can be listed on the screen if typing a ? mark on the prompt `Major element or alloy`. When a specific predefined alloy (instead of a major element) is selected, the major element is staked from the alloy definition and shown on the screen (with a message like `Alloy found with major element NI`). You can only specify alloying elements and the compositions (weight percent or mole percent). Typing a ? at any of the prompts for the alloying element names, e.g. `1st alloying element`, `2nd alloying element`, lists all the alloying elements and the composition limits in the alloy. If the composition of an alloying element is outside of its limit, there is a message (such as `Amount above limit: 30.0000`) and a prompt `Override limit ? /N/`. If you decide to enforce the override by answering `Y` on this prompt (i.e. accepting the over-limit alloying composition), another warning message (such as `Amount of major element below limit: 70.0000`) and prompt `Override limit ? /N/`. Then further decide if enforcing the overriding: if `Y` then accepting the major element's composition below the limit; if `N` then using the predefined

Syntax	DEFINE_MATERIAL
	major element composition limit.

DELETE_INITIAL_EQUILIBRIUM

Delete ONE specific initial equilibrium point or ALL of the initial equilibria. The initial equilibria are used as starting points for all the sub-sequential MAP and STEP calculations.

Also see *ADD_INITIAL_EQUILIBRIUM* on page 119.

Syntax	DELETE_INITIAL_EQUILIBRIUM
Prompt	`NUMBER /ALL/: <NUMBER OF AN INITIAL EQUILIBRIUM>`
	Specify the number of an initial equilibrium (as a specific digit e.g. 3, or ALL) to be deleted from the POLY3 workspaces. It is recommended to use *LIST_INITIAL_EQUILIBRIA* on page 157 to figure out the numbers for all the existing initial equilibrium points that have already been added (*manually* through *ADD_INITIAL_EQUILIBRIUM* on page 119, or *automatically* by some other POLY commands) and stored in the current POLY3 workspace. By default, ALL the initial equilibrium points are deleted.

DELETE_SYMBOL

Delete symbols (i.e. constants, variables, functions or tables. These symbols are entered with *ENTER_SYMBOL* on page 72.

Syntax	DELETE_SYMBOL
Prompt	`NAME: <NAME OF A SYMBOL>` Specify the name of the symbol to be deleted. Only one symbol can be deleted each time.

ENTER_SYMBOL

The information about this command is specific to the Thermo-Calc POST and POLY modules in Console Mode.

Symbols are a useful feature of the POLY and POST modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C_E command), stepping calculation (enforced by the command *STEP_WITH_OPTIONS* on page 172) or mapping calculation (enforced by *MAP* on page 158). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using *EVALUATE_FUNCTIONS* on page 155 before showing the corresponding values in the calculated equilibrium state.

The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.

Also see *ENTER_SYMBOL* on page 72 for the GIBBS Module.

See example 44 in the *Console Mode Examples Guide*for an example of using variables and functions.

Syntax	ENTER_SYMBOL
Prompt	`CONSTANT, VARIABLE, FUNCTION OR TABLE? /FUNCTION/: <KEYWORD>` The `Keyword` can be specified as `CONSTANT`, `VARIABLE`, `FUNCTION` or `TABLE`. • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by `P0` after the command ENTER CONSTANT `P0=101325`. Defined constants can be used as values in condition assignments, for example, `SET-COND P=P0`. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an *EVALUATE_FUNCTIONS* on page 155 command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET-CONDITION command. • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST. There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.
	`NAME: <NAME OF THE SYMBOL>` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names. You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, `TC=T-273.15` or `T_C=T273.15` which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.

Syntax	ENTER_SYMBOL
	For different types of symbol (constant, function, variable or table), the questions have different prompts.

	`FUNCTION: <DEFINITION FOR A FUNCTION OR VARIABLE>`
	Functions and *variables* are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).
	Unary functions like `LOG`, `LOG10`, `EXP`, `SIN`, `COS` and `ERF` can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing <Enter> at the next prompt).
	Examples of function expressions:
	• `GM(LIQUID)`: The Gibbs energy of liquid per mole component
	• `H.T/4.184`: The heat capacity of the system in calories
	• `ACR(CR)/X(FCC,CR)`: The activity coefficient for Cr in FCC
	• `T-273.15`: The temperature in Celsius
	`&: <CONTINUATION OF THE DEFINITION FOR THE SYMBOL>`
	The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.

	`VALUE: <VALUE FOR A CONSTANT>` A *constant* can only be assigned a numeric value once.
	`VALUE OR EXPRESSION: <VALUE OF EXPRESSION FOR A VARIABLE>` A *variable* can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.

	`VARIABLE(S): <VARIABLE(S) IN A TABLE>`
	A *table* consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.
	Example:
	`ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)`
	Which means that the table called K contains four columns, i.e. the temperature, the mole

Syntax	ENTER_SYMBOL
	fractions of C and Cr in the LIQUID phase, and the activity of C. To show the temperature in Celsius in a table, give the command ENTER FUNCTION `TC=T-273`; and then use the symbol `TC` in the table. `& <CONTINUATION OF THE DEFINITION FOR THE TABLE>` The ampersand `&` means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press <Enter> again.

EVALUATE_FUNCTIONS

The value of one or more or all entered functions or variables are evaluated and listed.

Syntax	EVALUATE_FUNCTIONS
Prompt	`NAME(S): <NAME(S) OF DEFINED FUNCTION(S)>` The names of one or more entered functions or variables must be specified. By typing a wildcard *, all functions and variables are evaluated. Variables are evaluated only if these are explicitly named.

LIST_AXIS_VARIABLE

Syntax	LIST_AXIS_VARIABLE
	Lists all the axis variables for a stepping or mapping calculation that have already been set by *SET_AXIS_VARIABLE* on page 164.

LIST_CONDITIONS

All the conditions that are set by the command SET_CONDITION and the command-sequence CHANGE_STATUS PHASE =FIXED <0 or 1 or alike>, are listed. The current conditions are also listed by the command LIST_EQUILIBRIUM. The degree of freedom in the defined system is also shown up. If this is zero, you can perform a COMPUTE_EQUILIBRIUM command. If it is larger than zero, some more conditions are required, and you must further set additional ones, using *SET_CONDITION* on page 165 or *CHANGE_STATUS* on page 135. If it is negative, a user has defined too many conditions and needs to take away the unnecessary ones, using the SET_CONDITION command (with a value of NONE for the to-be-deleted condition) or CHANGE_STATUS command (i.e. changing a FIXED status of a phase to another type of phase status, ENTERED or DORMANT or SUSPENDED).

Syntax	LIST_CONDITIONS

Example	`P=100000, T=800, N(NI)=1E-1, N=1`
	`FIXED PHASES`
	`FCC_A1=1 LIQUID=0   DEGREE OF FREEDOM 0`

LIST_EQUILIBRIUM

The result (always in SI units) from the last calculated equilibrium is listed on screen or in a textual file.

You can also execute this command if no calculation is made or if the calculation fails. It is your responsibility to interpret the results accordingly.

Syntax	LIST_EQUILIBRIUM
Prompt	`OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME>` The name of the text file where the list of the calculation results shall be written.
	`OPTIONS /VWCS/: <OPTION(S)>` Select the output units and formats by optionally specifying a combination of these letters. • *Fraction order:*`V` means VALUE ORDER; `A` means ALPHABETICAL ORDER. • *Fraction type*: `W` means MASS FRACTION; `X` means MOLE FRACTION. • *Composition*: `C` means only COMPOSITION; `N` means CONSTITUTION and COMPOSITION. • *Phase*: `S` means including only STABLE PHASES; `P` means including ALL NON-SUSPENDED PHASES.
	Default options are `VWCS`. If the output fraction type should be in mole fraction (rather than mass fraction), then give `VXCS` or type `X` (implying that in this case the options V, C and S are accepted as the listing manners for fraction order, composition and phase). If accepting all the default options, or if accepting all the altered options that had already changed when using this command previously, you can type `L_E,,,` or `LIST_EQUILIBRIUM ,,,` LIST_EQUILIBRIUM displays ORD (ordered) or DISORD (disordered) (when available). See *CHANGE_LEGEND* on page 193 for details.

LIST_INITIAL_EQUILIBRIA

List all the equilibria added with *ADD_INITIAL_EQUILIBRIUM* on page 119.

Syntax	LIST_INITIAL EQUILIBRIA
	All the initial equilibria are used for the MAP (and STEP) calculations.

LIST_STATUS

In the POLY module, list the status of components, species or phases.

Syntax	LIST_STATUS
Prompt	Specify what to list: `OPTION /CPS/: <KEYWORD(S)> KEYWORD    =   C OR P OR S,OR ANY COMBINATION` • `C` means list component status • `P` means list phase status • `S` means list species status • `CS` for both components and species Default is `CPS`.
	The results depend on the key word specified in the options for *CHANGE_STATUS* on page 59, a table with the current status of phases or species or components, or the combinations, is shown: • For components, the statuses and reference states are listed. • For species, only the status is listed. • For ENTERED and FIXED phases, the status, driving forces and equilibrium amounts are listed.
	✎ The metastable phases are listed in descending order of stability. To avoid long outputs only 10 metastable phases (in ENTERED status) are listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed.

LIST_SYMBOLS

For both the POLY and POST modules, list the definitions for all constants, functions, variables and tables.

In order to find the value of a function or variable, use *SHOW_VALUE* on page 172 or *EVALUATE_FUNCTIONS* on page 155. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %.

LOAD_INITIAL_EQUILIBRIUM

Copies all conditions and calculated results from a specific added initial equilibrium to the current equilibrium. The current conditions and calculation results are lost, and the newly loaded initial equilibrium point gets into the POLY workspace.

Syntax	LOAD_INITIAL_EQUILIBRIUM
Prompt	`NUMBER: <NUMBER OF AN INITIAL EQUILIBRIUM>` Specify the number of an initial equilibrium to be loaded as current. The number can be found with *LIST_INITIAL_EQUILIBRIA* on the previous page.

MAP

This command starts the mapping procedure for making a calculation of phase diagrams in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

Syntax	MAP
	A phase diagram consists of mapped phase boundary lines/curves; on one side of each such phase-boundary line/curve, the amount of one specific stable phase is zero (i.e. the zero-fraction lines). From a single MAP calculation, many different types of phase diagrams in the defined multicomponent heterogeneous system can be plotted, with some desired properties (that vary along the calculated phase-region boundaries) plotted as X/Y-axis variables. All different types of phase diagrams are generated by the mapping calculations through this command.

Normally, you need to have calculated at least one initial equilibrium point and have also defined at least two independent varying variables (i.e. the controlling conditions in the system) that are set with *SET_AXIS_VARIABLE* on page 164. You can also have three, or four or maximum five independent varying variables that are defined by the SET_AXIS_VARIABLE command).

This lists the current values of each of the independent axis variables for each of the calculated equilibrium points along each of the mapped phase boundaries, and also lists the corresponding information when the set of stable phases changes.

The Global Minimization Technique is by default enforced in this command while it can be disabled if having decisively switched it off (or possibly in some special modules) through changing the minimization option using the *ADVANCED_OPTIONS* on page 125 → MINIMIZATION_OPTION command-sequence. You can choose how often to do a Global Minimization test (via the Global Test Interval option) in the ADVANCED_OPTIONS STEP_AND_MAP command-sequence.

During a MAP calculation, the values of mapped axis-variables for presenting each phase boundary (lines/points) of the calculated phase-regions are listed, and the corresponding stable-phase sets are shown up. You can terminate the mapping of a line by pressing a single CTRL-A (Windows) or CTRL-C (Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at a certain stage during a calculation procedure enforced by this command, these messages display on screen:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30   to hardware
precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command *SET_NUMERICAL_LIMITS* on page 237 to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

In particular, for phase diagrams with tie-lines in the plane (i.e. most binary systems and ternary isotherms), there is a MAP procedure which checks for the best phase to use as axis variables in order to ensure reasonable increments between the tie-lines. This produces smoother curves and also gives a better stability in finding adjacent phase-regions.

Complex miscibility gaps of various solution phases are automatically detected during a mapping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a Global Test Interval value and confirming the `Automatically add initial equilibria` in the ADVANCED_OPTION STEP_AND_MAP command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can start calculating from high temperatures in an austenitic steel (metallic FCC_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC_A1 miscibility-gap, often (while not always) being referred to as `FCC_A1#2`, `FCC_A1#3`, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC_A1 phase and later also stable. The advanced mapping procedure (enforced by the Global Minimization Technique) inside the Thermo-Calc software (both the Console Mode and Graphical Mode) can efficiently and effectively handle complex miscibility gaps in multicomponent heterogeneous systems.

To get a complete phase diagram, sometimes it may be necessary to have multiple starting equilibrium-points, and/or to have added multiple initial-equilibrium points (through *ADD_INITIAL_EQUILIBRIUM* on page 119) inside various phase-region boundaries under certain direction(s).

POST

Syntax	POST
	Switches to the post-processor (the POST module), which has its own command repertoire.
	➲ See *POST Commands* on page 188 for all details.

READ_WORKSPACES

The POLY3 and GIBBS workspaces and the calculated results from the MAP and STEP commands can be READ from a file where they are saved with *SAVE_WORKSPACES* on page 30. Such an *.POLY3 file is not printable.

Syntax	READ_WORKSPACES
Options	`File name` is the name of a saved POLY3-file where the POLY3 and GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default *.POLY3 (Windows) or *.poly3 (Linux), otherwise type the whole POLY-file name. A window opens so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** (i.e. POLY3) cannot be changed. Click **Open** to open the POLY3 and GIBBS workspaces from the saved *.POLY3 file.
	When reading back an original POLY3 workspace that has already been saved as an *.POLY3 file in the current Thermo-Calc (Console Mode) run or had been read from an existing POLY3 file under the current work area, while some additional changes in the settings may be made but do not need to be kept in further steps in the current Thermo-Calc (Console Mode) run or any diagram is plotted in the POST module, you can type `READ,,` or `READ_WORKSPACE ,,`

RECOVER_START_VALUES

Syntax	RECOVER_START_VALUES
	Recovers the start values in equilibrium calculations.

REINITIATE_MODULE

Ensures that the whole POLY module (and thus the entire POLY workspace) is reinitiated to the state as it was when first entered.

Syntax	REINITIATE_MODULE
	All the defined components, defined conditions, changed status, entered symbols, defined independent axis-variables, calculated starting equilibrium-points, added initial equilibrium points, stepped/mapped equilibrium data, and so forth, are removed completely. The saved file name is restored to the default.

SAVE_WORKSPACES

Thermo-Calc allows saving the current status and workspaces of the program, including thermodynamic data, conditions, options and results from a single, stepping or mapping calculation on an *.POLY3 file. Do this for later use or when you need to terminate the current Thermo-Calc (Console Mode) run.

The POLY3 and GIBBS workspaces are saved on a file with this command. In the GIBBS workspace, all thermochemical data are stored. In the POLY3 workspace, all thermochemical data, all the last set of conditions and equilibrium state, changed status, entered symbols, advanced options, defined stepping/mapping variables, added initial equilibria, stepped/mapped results, etc., are stored, so it also contain the GIBBS workspace. After a SAVE_WORKSPACE command, you can always come back to exactly the state you had when you issued the SAVE_WORKSPACE command by giving a READ_WORKSPACE command.

After saving the POLY3 and GIBBS workspaces on a file, you can leave the program and at a later time READ the file and continue from the saved state.

A STEP or MAP command automatically saves the work file with the most lately specified name. Do not SAVE after a MAP or STEP.

The results from the STEP or MAP commands are destroyed by the SAVE_WORKSPACE command. You may append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

You may append several results by STEP or MAP without destroying the previous results but the SAVE command erases them all. To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

When you go to a response-driven module such as POTENTIAL or SCHEIL for example, a workspace file is automatically opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings is saved. The file is saved in the current working directory, and is named after the name of the module that created it. For example, the POTENTIAL module saves a workspace file called POT.POLY3 (or POT.poly3 in Linux); the POURBAIX module saves a file called POURBAIX.POLY3; etc.

Syntax	SAVE_WORKSPACES
Options	A `file name` must be specified. The default extension of the POLY workspace file is *.POLY3 (Windows) or *.poly3 (Linux), while you can have any other extension. A **Save** window displays, so that the path (in the **Save in** field) and **File** name can be specified. The file type (i.e. POLY3) in the **Files of type** cannot be changed. ✎ When saving a POLY3 workspace under a name that already exists under the current work area, which is saved by default (after running a special module, e.g. BIN, TERN, POT, SCHEIL and POURBAIX) or in an earlier stage of the current Thermo-Calc (Console Mode) run or in a previous run (which is READ into the current POLY3 workspace), you can type SAVE,,y or `SAVE_WORKSPACE ,,y`. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.

SELECT_EQUILIBRIUM

If you create more than one initial equilibrium (during data-assessments using the PARROT/ED_EXP modules), you can switch between them using this command.

Syntax	SELECT_EQUILIBRIUM
Prompt	`NUMBER /NEXT/: <CHOICE ON EQUILIBRIUM>` Answer `FIRST`, `LAST`, `NEXT`, `PREVIOUS` or `PRESENT`. Most commands affect only the `PRESENT` equilibrium. However, the commands *REINITIATE_MODULE* on the previous page and *DEFINE_COMPONENTS* on page 143 remove all the stored equilibria.

SET_ALL_START_VALUES

Set start values, e.g. if the calculation fails or if you have a miscibility gap or ordering. If temperature and pressure are not conditions, you are asked for values of them. Then for each phase prompt on if it should be stable and on its constitution.

Syntax	SET_ALL_START_VALUES
	`T /XXXX/: <TEMPERATURE IN K>` If the temperature is not a condition, supply a guess of its final value (in K).
	`P /100000/: <PRESSURE IN PA>`

Syntax	SET_ALL_START_VALUES
	If the pressure is not a condition supply a guess of its final value (in pa).
Prompts	`AUTOMATIC START VALUES FOR PHASE CONSTITUTIONS? /N/: <Y, N OR F>` Answer `N` (the default), `Y` or `F` (for force). The reason for the `F` option is that in some cases the calculation has failed because impossible conditions are set, e.g. `W(C)=1.5 [W(C)` is mass fraction and must thus be less than unity]. The program tries to fulfil this condition by putting maximum amount of carbon in all phases, but can fail anyway. When you detect the error and set `W(C) to 0.015`, the calculation may still fail because it could start from the previous values. To get back to 'fresh' start values, give the answer `F` for `FORCE`. If `Y` this command immediately terminates, and the program automatically sets the start values for phase constitutions in all possible phases. For `N` supply an initial amount of each entered phase and the major constituents or site fraction of each constituent.
	`SHOULD <PHASE> BE STABLE /N/: <Y/1 OR N/2>` A guess on if this phase should be stable or not is requested. All entered phases are prompted for this question and next two. You cannot have more phases stable than you have components, but at least one (which dissolves all constituents) must be set as stable. For backward compatibility, this question can be answered by 1 (for Yes) or 0 (for No). The `phase` name may have a hash sign # followed by a digit, e.g. `BCC_A2#2`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign.
	`MAJOR CONSTITUENT(S): <NAME OF MAJOR CONSTITUENT(S) IN THE PHASE>` The constituent with the largest fraction in the phase should be specified. If there are more than one constituent with a large fraction, give them all on the same line. If the default major constituents should be used answer with an asterisk (*). By giving $ the constitution is not changed. If there should be no major constituent give NONE and or if the major constituent(s) are improperly specified, you are asked for individual fractions in the phase.
	`Y(<PHASE>,<CONSTITUENT>) /.XXXXXXXXXX/: <.YYYYY>` The current value (`.XXXXXXXXXX`) is default. You can accept the default by pressing

Syntax	SET_ALL_START_VALUES
	<Enter> or give a new value (`.YYYYY`). The phase name or constituent name may have a hash sign # followed by a digit, e.g. `Y (BCC_A2#2,FE), Y(BCC_A2#2,C#2)`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign. For phases with sublattices, the constituents in sublattice 2 or higher is also be suffixed with a hash sign # followed by a digit.

SET_AXIS_VARIABLE

In order to calculate a diagram, set at least one axis variable in a stepping calculation, or at least two axis variables in a mapping calculation. For property diagrams, one axis is enough; for phase diagrams two or more are necessary. Any condition that can be set to calculate an equilibrium can be used as an axis variable (with its lower and upper limits and step length) by using the SET_AXIS_VARIABLE command, and the POLY program does, after a STEP or MAP command, vary the value of the condition between the limits set on its related axis variable. As an extraordinarily unique and powerful feature of the Thermo-Calc software, up to five independent axis variables can possibly be used in a mapping calculation of a multicomponent heterogeneous system; however, the axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.

Syntax	SET_AXIS_VARIABLE
Prompts	`AXIS NUMBER /#/: <AN AXIS NUMBER>` Specify a number between 1 and 5. The axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.
	`CONDITION /NONE/: <ONE CONDITION>` Here the condition that should be varied along the axis must be given. The condition is specified as in *SET_CONDITION* on the next page, for example `W(C)` for mass fraction of carbon. By accepting `NONE`, the axis is removed.
	`MIN VALUE /0/: <MIN VALUE>` Specify the minimum value of the axis condition.
	`MAX VALUE /1/: <MAX VALUE>` Specify the maximum value of the axis condition.
	`INCREMENT /.025/: <STEP LENGTH>` Specify the maximum step length. By default, this is 1/40 of the total axis length.

You can give the SET_AXIS_VARIABLE command without having set a condition on the axis variable. Under such circumstances, the relevant condition is automatically created and the value set between the minimum and maximum axis limits; however, as a side effect, the POLY module creates two conditions, `P=1e5` and `N=1` (these have not been defined as a condition yet), in case you set an axis variable which is not already a condition.

You can use a logarithmic axis during calculations. This is useful for low fractions like in a gas phase where `1e-7` to `1e-2` might be an interesting range. The pressure is also suitable for logarithmic step. You specify the logarithmic axis by giving an asterisk * after the increment value.

The increment in this case is treated as a factor.

For example,

```
S-A-V 1 P 1E5 1E25 5*
```

This makes axis 1 a logarithmic axis where the difference between two calculated values makes a factor 5.

The factor must be larger than 1.0.

In some cases, such as when the DEFINE_DIAGRAM command is used or a special advanced module (e.g. BIN, TERN, POT, SCHEIL or POURBAIX) is called, some axis variables are automatically set by the program, not necessarily by this command.

SET_CONDITION

Specify the equilibrium conditions for the calculation. All kinds of state variables, as well as most of the M/W/V/F-suffixed state variables (for normalization) and R-suffixed state variables (with respect to chosen reference states), can be used as conditions. Beside temperature and pressure conditions, a multicomponent system can have mixed types of conditions; this brings the extreme flexibility and powerfulness to the complex calculations with the Thermo-Calc software system. You should repeat this command for a multicomponent system, till the degree of freedom in the defined system becomes zero. When a FIXED phase status is used on a specific phase (use *CHANGE_STATUS* on page 135), it is equivalent to one condition (implying that particular phase is stable in the defined system).

Syntax SET_CONDITION

Each condition must be given explicitly, but can be given on the same line (separated by a comma (,) or an empty space) or on separate lines with each one started with the command.

Example

```
SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,CR)=.22, ACR(N)=.2
```

or

```
SET_COND T=1273, P=1E5
SET_COND W(C)=.0015, X(LIQ,CR)=.22 ACR(N)=.2
```

In this example, the temperature is set to 1273 K, the pressure to 1 bar (1E5 Pascal), the mass (weight) fraction of C to 0.0015 and the mole fraction of Cr to 0.22 and the activity of N to 0.2.

Prompt

`STATE VARIABLE EXPRESSION: <STATE VARIABLE NAME OR LINEAR EXPRESSION> OR A LINEAR EXPRESSION OF STATE VARIABLES.`

Some of the state variables that can be used in conditions are:

- `T`: temperature in the system (in K)
- `P`: pressure in the system (in Pascal)
- `N`: system size (mole number in moles)
- `B`: system size (mass in grams)
- `N(<component>)`: mole number of a component in the system
- `X(<component>)`: mole fraction of a component in the system
- `W(<component>)`: mass fraction of a component in the system
- `ACR(<component>)`: activity of a component in the system
- `MUR(<component>)`: chemical potential of a component in the system
- `X(<phase>,<component>)`: mole fraction of a component in a phase
- `W(<phase>,<component>)`: mass fraction of a component in a phase
- `ACR(<species>,<phase>)`: activity of a species in a solution phase
- `MUR(<species>,<phase>)`: chemical potential of a species in a solution phase
- `H`: enthalpy in the system (in J)
- `HM(<phase>)`: enthalpy of a phase (in J/mol)

Syntax	SET_CONDITION

There are many state variables that can be used in conditions. For more information, enter an `INFO STATE_VARIABLES` command. A condition is normally a value of a single state variable with its value.

Example

```
T=1273.15  P=1E5

X(C)=.002

W(CR)=0.5

ACR(CR)=0.85

X(FCC,C)=.001

H=-250000

HM(BCC)=-225000
```

A condition can also be a value of a linear expression involving more than one state variable. For example,

```
X(LIQ,S)-X(PYRR,S)=0
```

This means that it is a condition that the mole fraction of `S` component should be the same in the LIQUID and PYRRHOTITE phases. In practice, that should be the congruent melting point.

✎ After the equal sign only a numeric value is allowed in the expression.

`FACTOR: <A FACTOR FOR THE STATE VARIABLE, OR A CONTINUATION>`

This question means you did not answer the previous question. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:

```
2*MUR(FE)+3*MUR(O)=-35000
```

This means that it should be a condition that two times the chemical potential of `FE` plus three times the chemical potential of `O` should be -35000 J/mol.

`STATE VARIABLE: <A SPECIFIED STATE VARIABLE, OR A CONTINUATION>`

This question is prompted if a single state variable name has not given in either the prompt `State variable expression` or `Factor`, or a state variable expression is given but the expression is incomplete, for example, `T-` or `2*MUR(FE)+`, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable

Syntax	SET_CONDITION
	expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).
	`VALUE /X/: <A NUMERIC VALUE, A CONSTANT OR A VARIABLE>` The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value `NONE` means that the condition is removed; for example `T=NONE` takes away the temperature condition.

SET_INPUT_AMOUNTS

Specify how a system is made up from mixing of various substances. It is useful with a substance database. In the C-H-O-N system, you can, for example, give:

```
S-I-A N(H2)=10, N(H2O)=25, N(C1O2)=5, N(N2)=100
```

The POLY module automatically converts this into conditions for the current set of components. In the case when the elements are defined as the components, the command above is equivalent to

```
SET-CONDITION N(H)=70, N(O)=35, N(C)=5, N(N)=200
```

Syntax	SET_INPUT_AMOUNTS
Prompts	`QUANTITY: <N(<SPECIE>) OR B(<SPECIE>)>` You can give the amount also preceded with an equal sign `=` [e.g. `N(H2)=10` or `B (H2O)=1000`], or press <Enter> for the next prompt on the amount of the quantity.
	`AMOUNT: <VALUE OF THE QUANTITY>` Specify the numerical value of the quantity. You can give negative amounts in the SET-INPUT-AMOUNTS command.

SET_NUMERICAL_LIMITS

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by *COMPUTE_EQUILIBRIUM* on page 139, *STEP_WITH_OPTIONS* on page 172, *MAP* on page 158 or *ADVANCED_OPTIONS* on page 125), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30 to hardware
precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current Thermo-Calc (Console Mode) run, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	`MAXIMUM NUMBER OF ITERATIONS /200/: <XXX>` By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
	`REQUIRED ACCURACY /1E-6/: <YYY>` This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
	`SMALLEST FRACTION /1E-12/: <ZZZ>` This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is `1E-12` for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as `1E-30` (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system).
	`APPROXIMATE DRIVING FORCE CALCULATION FOR METASTABLE PHASES /Y/: <Y OR N>` Normally the POLY module only requires that the set of stable phases is in equilibrium in order to terminate the iterations. The metastable phases are included in all iterations but these may not have reached their most favourable composition and thus their driving forces may be only approximate [corresponding to `Y`]. You can also force the calculation to converge for the metastable phases by answering `N` if it is important that these driving forces are correct, which may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.

SET_REFERENCE_STATE

The reference state for a component is important when calculating activities, chemical potentials and enthalpies. The reference state for a component is determined by the database. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state. All data in all phases where this component dissolves must use the same reference state. However, different databases may use different reference states for the same element. Thus you must be careful when, for example, mixing data from different databases.

By default, activities, chemical potentials, etc. are computed relative to the reference state used by the database and this may thus differ depending on the database. With this command select the reference state for a component if the reference state in the database does not suit.

You can set the reference state for a component as `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys that is dominated by the component). Under such a case, the temperature and pressure for the reference state is not needed and thus is not prompted.

In order to specify conditions in the specified reference state, you can append an R to the state variables. Thus, AC is the activity (of a system component or of a species in a phase) with respect to the default reference state, and ACR is the activity with respect to the selected reference state; MU is the chemical potential of a system component with respect to the default reference state, and MUR stands for the chemical potential with respect to the selected reference state. The AC and ACR variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. LNAC(Fe), LNACR(C), LNAC(O2,GAS), LNACR(O2,GAS).

Syntax	SET_REFERENCE_STATE
Prompts	`COMPONENT: <NAME OF THE COMPONENT>` The name of the component must be given.
	`REFERENCE PHASE: <NAME OF A PHASE USED AS THE NEW REFERENCE STATE>` The `Name of a phase`, that must be either ENTERED or DORMANT or SUSPENDED, must be given here. The component must, of course, be a constituent of this phase. For a phase to be usable as reference for a component the component need to have the same composition as an end member of the phase. The reference state is an end member of a phase. For example, in the Fe-C system, BCC can be a reference state for Fe but not for C since BCC cannot exist as pure C. If a component has the same composition as several end members of the chosen reference phase, then the end member is selected that at the specified temperature and pressure has the lowest Gibbs energy. For example, setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently become the reference state. The actual calculation of the reference state is only performed when SET_REFERENCE_STATE is executed. For example, if GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1.
	`TEMPERATURE /*/: <TEMPERATURE FOR THE REFERENCE STATE>`

Syntax	SET_REFERENCE_STATE
	Select the temperature (in K) for the reference state. The wildcard value * means the current temperature is used for the calculation.
	`PRESSURE /1E5/: <PRESSURE FOR THE REFERENCE STATE>` Select the pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for the calculation.

	Examples
	`S-R-S Fe SER`
	`S-R-S Cr FCC * 100000`
	`S-R-S H2O AQUEOUS * 100000`
	`S-R-S ZE REF_ELECTRODE * 100000`

SET_START_CONSTITUTION

This command is similar to *SET_ALL_START_VALUES* on page 162, but is used for an individual phase that may have a wrong constitution.

Syntax	SET_START_CONSTITUTION
Prompts	`PHASE NAME: <NAME OF A PHASE, AND POSSIBLE MAJOR CONSTITUENT(S)>` Specify the name of a phase for which the constitution shall be set. If there is a major constituent of the phase, you must specify this on the same line as the phase name. By giving an*, select the default major constituents. A $ means keeping the same constitution, and `NONE` means to give individual site-fractions.
	`Y(<PHASE>#<COMPOSITION_SET>,<CONSTITUENT>#<SUBLATTICE>) /XXX/: <SF>` The site fraction (`SF`) of the constituent shall be given. The default value `xxx` is the last calculated one.

SET_START_VALUE

Set a start value of an individual variable.

This command is not often required as the automatic start values can be handled for most problems.

Syntax	SET_START_VALUE
Prompts	`STATE VARIABLE: <NAME OF A STATE VARIABLE>` The state variable must be given.
	`VALUE` Specify the value to be assigned the state variable as start value.

SHOW_VALUE

Show the current value of any state variable, function or variable.

Syntax	SHOW_VALUE
Prompt	`STATE VARIABLE OR SYMBOL: <NAME(S) OF STATE VARIABLE(S) OR SYMBOL(S)>` A single or several state variables or symbols (entered functions or variables) can be specified.
	The wildcard * can be used to denote all phases or all components. You can use the dollar-sign $ to denote all stable phases. Thus, the command SHOW W (*,*)lists the mass fraction of all phases, whereas `SHOW W($,*)` lists the mass fraction of all stable phases. If you SHOW a function, all functions are evaluated using the current values of the state variables. But if you SHOW a variable, it retains its value from the time it was ENTERED or last EVALUATED. Therefore to save a value from one calculation to another, ENTER it to a variable. This is frequently done in the PARROT module to transfer values between equilibria.

STEP_WITH_OPTIONS

Initiates the stepping procedure to make a calculation of property diagrams in a multicomponent heterogeneous system. A property diagram is usually stepped under one defined independent stepping axis-variable, and is often constructed by the defined independent mapping axis-variable against a chosen property (for the system, or for a specific phase, or for a certain species).

A property diagram consists of property lines that change (normally) along with the stepping axis-variable. From a single STEP calculation, many different types of property diagrams in the defined multicomponent heterogeneous systems can be plotted. Various types of property diagrams are generated by the stepping calculations through this STEP_WITH_OPTION command

Normally, before it can be invoked, you must have already calculated an initial equilibrium point and have also set one independent varying variable (i.e. the controlling condition in the system) using *SET_AXIS_VARIABLE* on page 164.

The Thermo-Calc Console Mode lists the current values of the axis variable for each calculated equilibrium, as well as the corresponding information when the set of stable phases changes.

The Global Minimization Technique is by default enforced in this command (STEP), while it can be disabled if having decisively switched it off by a user (or possibly in some special modules) through changing the minimization option using the *ADVANCED_OPTIONS* on page 125 → MINIMIZATION_OPTION command-sequence.

You can choose how often to do a Global Minimization Test (via the `Global Test Interval` option) in the `ADVANCED_OPTIONS STEP_AND_MAP` command-sequence.

- NORMAL: Allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable).
- INITIAL_EQUILIBRIA: An initial equilibrium is stored at each calculated equilibria. It is intended to generate a matrix of calculated initial equilibria, first stepped under a STEP INITIAL_EQUILIBRIA command-sequence and then repeated by another STEP NORMAL command-sequence (or even continued by a MAP command). For example, you can first use the temperature condition as the stepping axis-variable, and give a STEP INITIAL_EQUILIBRIA command sequence; this calculates a number of initial equilibrium points and automatically ADDs each one as an initial equilibria for another STEP NORMAL command-sequence (or even for a MAP command). Before the second STEP command (i.e. the STEP NORMAL command-sequence), you can alternatively chose a compositional condition as the new stepping axis-variable; then the STEP NORMAL command-sequence uses those created starting equilibrium points (at different temperatures) and steps in such a new compositional variable. As a result, these two sequential STEP commands together give a matrix of values. Actually, you can carry this option even deeper.
- SEPARATE_PHASES: Each of the entered phases are calculated separately and in parallel at each step, i.e. all the phases are calculated for the same composition (if the phases exist for that composition). In this way, you can calculate how the Gibbs energy for a number of phases varies for varying compositions; and this option is particularly useful for calculating Gibbs energies for complex phases with miscibility gaps and for ordered phase which is never disordered (e.g. SIMGMA-phase, G-phase, MU-phase or alike).

However, this option may sometimes be unable to find all the ordered phases and their disordered pairs during a STEP SEPARATE_PHASES calculation; and it is thus recommended to always use the newer ONE_PHASE_AT_TIME option instead, for STEPPING heterogeneous systems with both ordered phases and their disordered pairs.

- ONE_PHASE_AT_TIME: The stepping calculation is conducted for only one phase at a time individually (stepped over the whole stepping variable range), but the stepping is repeated for all the entered phase in the defined system. This new option is particularly useful for properly stepping in composition for an equilibrium heterogeneous system with both ordered phases and their disordered pairs, because of that, instead of calculating for the same composition for each of the phases at each composition step, it at least starts the stepping in each of the phases in the default most-stable compositions (the major constitutions). Therefore, this option is always recommended for STEPPING heterogeneous systems with both ordered phases and the disordered pairs.
- EVALUATE: The variables given are evaluated after each step, which may change other conditions. This option is useful for performing the Ordinary ScheilGulliver Approach (non-equilibrium transformations) for simulating alloy solidifications without back diffusion of fast-diffusing interstitial components in solid phases. However, users are always recommended to go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations in a much easy, straightforward and automatic way.
- MIXED_SCHEIL: A stepping calculation designed for the Extended Scheil-Gulliver Approach (partial-equilibrium transformations) to simulate alloy solidifications with back-diffusion of one or more fast-diffusing interstitial components (such as C, N, O, S, etc.) in solid phases is performed. However, you are always recommended to go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations in a much easy, straightforward and automatic way.
- T-ZERO: T0 (T-zero) lines in a diffusionless transformation [where two specific partially-equilibrated phases have the same Gibbs energy] are calculated along a composition variable (set as the stepping variable).
- PARAEQUILIBRIUM: The paraequilibrium state in a partly partitionless transformation [under which two partially-equilibrated phases have the same chemical potential (but different contents) for one or more interstitial components, such as C, N, O, S, etc.] is calculated along varied temperature or along a composition variable (of the matrix or one substitutional component).

Syntax	step_with_options
Prompt	`OPTION? /NORMAL/: <A CHOSEN OPTION, N OR I OR S OR O OR E OR M OR T OR P>`
Options	**Choose from these options**
`NORMAL`	Allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable). By repeating the STEP NORMAL command-sequence, you can make several stepping calculations while still keep all the stepping-calculation results in the same current POLY3 workspaces (saved in the same `RESULT.POLY3` file default-named by the program, or in the same `<MyName>.POLY3` file that is specified before the first STEP NORMAL command-sequence). Only when there is no SAVE_WORKSPACES command issued before the repeated STEP NORMAL command-sequence, such repeated stepped results can be restored into the same current POLY3 workspaces/file. Choose to alter one or more controlling conditions for calculating starting equilibrium point(s) and can also optionally change the independently-varying condition (stepping-variable) and its settings for the stepping. All such alternations/changes are properly stored into the current POLY3 workspaces/file. Therefore, with one or more repeated STEP NORMAL command-sequence (without any SAVE_WORKSPACES command in between for overwriting stepped results), it enables you to easily/efficiently generate some special types of property diagrams and even to plot special phase boundary lines on phase diagrams, as described below: Calculate/plot missing part(s) of a specific property [that are calculated under another controlling condition inside the range of the stepping-variable] on the same property diagram. Calculate/plot two or more sets of a specific property [that are calculated under different controlling conditions and stepped over the same stepping-variable range] on the same property diagram for the same system. Calculate some special phase-boundary lines [especially for some defined secondary phase transformations or alike, e.g. the BCC_A1 <--> BCC_B2 phase-boundary, or equal-Gm for two specific phases, or equal-fraction or equal-activity for a certain species in two specific phases, that shall be calculated under different controlling-conditions and also be stepped over different stepping variable(s)], and then plot (or impose) them onto a corresponding phase diagram (which can be resulted from several such STEP NORMAL calculations or even from a separate

Syntax	step_with_options
	MAP calculation) for the same system.
`INITIAL_ EQUILIBRIA`	An initial equilibrium stored at every step. This option has not been completely implemented yet. It is intended to make a stepping calculation by generating a matrix of calculated initial equilibria, first stepped under a STEP INITIAL_ EQUILIBRIA command-sequence and then repeated by another STEP NORMAL command-sequence (or even continued by a MAP command). For example, you can first use the temperature condition as the stepping axis-variable, and give a STEP INITIAL_EQUILIBRIA command-sequence; this calculates a number of initial equilibrium points and automatically ADDs each one as an initial equilibria for another STEP NORMAL command-sequence (or even for a MAP command). Before the second STEP command (i.e. the STEP NORMAL command-sequence), you can chose a compositional condition as the new stepping axis-variable; then the STEP NORMAL command-sequence uses those created starting equilibrium points (at different temperatures) and steps in such a new compositional variable. As a result, these two sequential STEP commands together give a matrix of values.
`SEPARATE_PHASES`	Each phase is calculated separately. This option performs a stepping calculation in which all the entered phases in the system are calculated separately and in parallel at each step, i.e. all the phases are calculated for the same composition (if the phases exist for that composition). In this way, you can calculate how the Gibbs energy for a number of phases varies for varying compositions. This option is useful when you want to plot `Gm` curves versus composition for a given temperature, particularly for calculating the Gibbs energy differences for phases with miscibility gaps and for ordered phase which is never disordered (e.g. SIMGMA-phase, G-phase, MU-phase or alike). However, this option may sometimes be unable to find all the ordered phases and their disordered pairs during a STEP SEPARATE_PHASES calculation procedure; and it is thus recommended to always use the newer ONE_PHASE_AT_TIME option instead, for STEPPING heterogeneous systems with both ordered phases and their disordered pairs.
`ONE_PHASE_AT_ TIME`	One phase calculated at a time and repeated for all entered phase. It allows a stepping calculation for only one phase at a time individually (stepped over the whole stepping variable range), but the stepping is repeated for all the entered phase in the defined system. The STEP ONE_PHASE_AT_TIME command-sequence properly STEP in composition for an equilibrium heterogeneous system with both ordered phases and their disordered pairs, instead of calculating for the same composition for each of the phases at each composition step, and it at least starts the stepping in each of the phases in their default most-stable compositions (the major constitutions). Therefore, this option is always recommended for STEPPING

Syntax	step_with_options
	heterogeneous systems with both ordered phases and their disordered pairs.
EVALUATE	Specified variables evaluated after each step. This is an advanced option for experts of Thermo-Calc, when additional conditions (rather than the stepping variable) should be changed during a stepping calculation. It allows a stepping calculation in a single axis with simultaneous evaluation of one or more variables after each step. As variables can be used as conditions, it means that you can change the conditions during the stepping. After a successful STEP EVALUATE calculation, you can go to the POST module to manually define and plot various desired property diagrams. Specify the prompt: `VARIABLE NAME(S): <VARIABLE NAME>` The names of the variables that shall be evaluated after each step must be typed here. During a STEP EVALUATE calculation in some earlier TCC versions, it used to calculate all kinds of property diagrams, phase fraction plots, etc., some problems may occur, especially when new phases want to appear. These problems are simplified by the general improvement of convergence but a number of additional fixes are added to the STEP EVALUATE command-sequence to handle the problems. The miscibility gap test is automatically used during stepping (see the command *ADVANCED_OPTIONS* on page 125) if a phase has two or more composition sets. The miscibility gap test means that you can now start calculating from high temperatures in a steel, where the MC carbide is not stable; and during a STEP EVALUATE calculation procedure, the MC carbide first becomes metastable with a composition different from the metallic FCC phase and later also stable. One good case of using this advanced option is described in the command *INFORMATION* on page 5 with the subject as SOLIDIFICATION (Solidification Path Calculations). With this option, you can simulate the Ordinary Scheil-Gulliver Solidification Processes (i.e. non-equilibrium transformations) by changing the overall composition to the new liquid composition after each step, but without considering back-diffusion of fast-diffusing interstitial components in solid phases. See example 30A in the *Console Mode Examples Guide*. It is recommended to go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations.

Syntax	step_with_options
`MIXED_SCHEIL`	Extended Scheil-Gulliver type solidification with back diffusion. This option leads to a stepping calculation (always with T as the stepping axis variable) for simulating Extended Scheil-Gulliver solidification processes (i.e. *partial-equilibrium transformations*) with considering back-diffusion of one or more fast-diffusing interstitial components (such as C, N, O, S, etc.) in formed solid phases; it also allows considering BCC-->FCC phase transformation (practically for steels) along the alloy solidification process. To ensure a successful stepping calculation of mixed Scheil-Gulliver simulation of solidification process of a defined alloy system with a certain initial overall composition, it is important to pay special attention to the following four aspects, before performing this advanced-option stepping calculation: For solution phases with possibility of miscibility gap existence, you have appropriately added the necessary composition set(s); You have already set the temperature condition as the stepping SET_AXIS_VARIABLE command, with a minimum and maximum temperature points as well as an appropriate s temperature step for the cooling process); It is equally important there must be a composition condition for each of the back-diffusion components (i.e. fast-diffusing interstitial components, such as C, N and/or other elements) that are already defined in terms of mole-fraction or mass-fraction, e.g. `X(C)` and `W(N)`. Otherwise, a stepping calculation with this option can fail. An initial equilibrium in which the LIQUID mixture phase is the only stable must be calculated [for this reason, it is always good to start with a relatively high temperature condition for the initial equilibrium calculation; and it is always necessary to reject or suspend the GAS mixture phase (if exists) before the C-E and STEP commands, to avoid its formation along with LIQUID]. In cases where fast-diffusing interstitial components are specified as back-diffusion components, there is a possibility to choose an option to `allow BCC>FCC` phase transformation (practically for steels) during the alloy solidification process. With this stepping calculation option, these prompts need to be specified: `FAST DIFFUSING COMPONENTS: <FAST DIFFUSION INTERSTITIAL(S)>` Specify one or more interstitial component(s) as the back-diffusion component(s). If there is only one fast-diffusing interstitial component (e.g. C or N), type its name at the prompt;

Syntax	step_with_options

If there are two or more fast-diffusing interstitial components (e.g. C, N and S), always type their names on the same line at once (separated by an empty space in between, e.g. C N S);

If there is no fast-diffusing interstitial component to be considered, type `NONE` to ignore back diffusion entirely, meaning a normal Scheil-Gulliver simulation is performed.

Such specified back-diffusion interstitial component(s) must be appropriately defined according to the phase constitution definitions of some major alloy solution phases (e.g. FCC, BCC, HCP, etc.): These are located on the interstitial/vacancy sublattices in such alloy solution phases; otherwise, such a Scheil-Gulliver simulation may not make sense at all.

```
ALLOW BCC -> FCC ? /Y/: <Y OR N>
```

Type `Y` (or press <Enter> to accept the default) or `N` to allow or not allow the `BCC-->FCC` phase transformation (which is usually a typical phenomenon along the cooling processes of steels/Fe-alloys).

During the STEP MIXED_SCHEIL calculation procedure, the simulated solidification path, including the locally-equilibrated phase assemblage (region), captured temperature condition (`T` in K), remaining liquid phase (`NL`, mole fraction), overall formed solid phases (`NS`, mole fraction) and latent heat formation (`NH`, J/mol) along the cooling process are shown after the information on starting temperature point of the alloy solidification process, e.g.

```
Solidification starts at  1743.15 K

Phase Region from   1.744150E+03 for:      LIQUID

Phase Region from   1.742525E+03 for:

     LIQUID

     FCC_A1#1

       1742.5250         0.9960          0.0040         -1.1824

       1742.4000         0.9795          0.0205       -202.1585
. . . . . .
Phase Region from   1.733150E+03 for:

     LIQUID

     BCC_A2

     FCC_A1#1
```

Syntax	step_with_options

	`1733.1500        0.3294        0.6707     -8032.6240`
	`1733.0250        0.3237        0.6763     -8095.1490`
	`. . . . . .`
	After a successful STEP MIXED_SCHEIL calculation, you can go to the POST module to manually define and plot various property diagrams for the alloy solidification process according to the chosen Scheil-Gulliver model, or to impose existing relevant experimental information or other types of calculated solidification results [e.g. Scheil-Gulliver simulation with or without considering fast-diffusing interstitial component(s), full-equilibrium approach, or Diffusion Module (DICTRA)-type simulation with moving-boundary conditions] onto the same plotted property diagrams. Normally, the solidus temperature (`T` in Celsius) is set as one of the axis variables (usually as Y-axis in most cases), while the other plotted quantity on the other axis can be the amount of overall formed solid alloy phases (`NS` in mole-fraction or `BS` in mass-fraction), the amount of remaining liquid phase (`NL` in mole-fraction or `BL` in mass fraction), the heat of latent along the solidification process (`NH` in J/mol or `BH` in J/gram), among many other properties in the solidified alloy phases or in the whole alloy system.
	However, you are always recommended to go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations in a much easy, straightforward and automatic way.

`T-ZERO`	T0 lines between two specific phases calculated This option allows a stepping calculation of the so-called T0 (T-zero) line in a *diffusionless transformation* [where two specific partially-equilibrated phases have the same Gibbs energy, along a composition variable which has already set as the stepping variable with *SET_AXIS_VARIABLE* on page 164.
	❗ The temperature condition cannot be set as the stepping variable if you want to make a STEP T-ZERO calculation.
	To ensure a successful calculation of T0 line between two specific phases after an initial equilibrium calculation in the current system, it is recommended to make a single T0 point calculation by the ADVANCED_OPTION T-ZERO command-sequence, prior to performing this STEP T-ZERO command-sequence, although this might not be always necessary for some systems.
	Specify these prompts:
	`NAME OF FIRST PHASE:  <PHASE A>`
	`NAME OF SECOND PHASE: <PHASE B>`

Syntax	step_with_options
	The names of the two target phases, for which the Gibbs energies equal to each other at each point on the T0 line, must be typed at the above two prompts subsequently. During the STEP T-ZERO calculation procedure, the calculated T0 values are shown after the corresponding scanned conditions (of the stepping composition variable), e.g.

```
Phase Region from   1.000000E-01 for:
     BCC_A2
     FCC_A1
   1.000000E-01         940.24
   9.250000E-02         941.20
   . . . . . .
   2.500000E-03         977.61
   7.500000E-09         979.34
Phase Region from   1.000000E-01 for:
     BCC_A2
     FCC_A1
   1.000000E-01         940.24
   1.075000E-01         939.62
   . . . . . .
   2.950000E-01        1084.87
3.000000E-01        1080.99
```

	After a successful STEP T-ZERO calculation, you can go to the POST module to plot the T0 line against the stepping composition variable or another varying axis, or to impose the calculated T0 line onto a normal phase diagram [normally plotted as a `T-X` isopleth]. See examples 23 and 41 in the *Console Mode Examples Guide*.
PARAEQUILIBRIUM	Paraequilibrium state between two specific phases is calculated with this. It allows a stepping calculation of so-called paraequilibrium lines in a partly partitionless transformation between two specific partially-equilibrated phases in an alloy system where the chemical potential for one or more fast-diffusing interstitial components but not for the substitutional components in two specified phases are equal.

Syntax	step_with_options
	Therefore, the STEP PARAEQUILIBRIUM command-sequence ensures that the two partially equilibrated phases have the same chemical potential (but different contents) for one or more fast-diffusing interstitial components (such as C, N, O, S, etc., as individual or combined)], along varied temperature or along a composition variable (of the matrix or one substitutional component) which has already set as the stepping variable with *SET_AXIS_VARIABLE* on page 164. More than one interstitial components can be treated as fast-diffusion species (such as C, N, O, S, etc., as individual or combined) in a paraequilibrium stepping calculation. ✎ The composition condition for the interstitial components cannot be set as the stepping variable if you want to make a STEP PARAEQUILIBRIUM calculation. To ensure a successful stepping calculation of paraequilibrium states between two specific phases in a defined alloy system, it is important to first make a starting-point equilibrium calculation with an initial overall composition in the current system before performing this advanced-option stepping calculation; however, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable. The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true for cases where there are more than one interstitial components to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviours as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state. Always check if the chosen `phaseA` and `phaseB` have the exact same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions). Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and staring bulk composition for the system. Always set the status of the chosen interstitial components as SPECIAL using the command:

Syntax	step_with_options

```
CHANGE_STATUS COMPONENT <interstitial component> = SPECIAL
```

By doing this, you get a clear picture on u-fractions of various substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from the paraequilibrium calculations are u-fraction related quantities.

Always make a single-point paraequilibrium calculation by the command-sequence of ADVANCED_OPTIONS PARAEQUILIBRIUM, prior to performing this STEP PARAEQUILIBRIUM command-sequence, although this might not be always necessary for some systems.

With this stepping calculation option, these prompts need to be specified:

```
NAME OF FIRST PHASE:  <PHASE A>
NAME OF SECOND PHASE: <PHASE B>
```

The names of the two target phases `A` and `B`, between which the paraequilibrium states establish, must be typed at the above two prompts subsequently or on the same (first) line at once (separated by an empty space, e.g. `FCC BCC`, `FCC#2 M23C6`).

> ❗ It is important to understand that this is the calculation of a paraequilibrium state between the two specified phases.

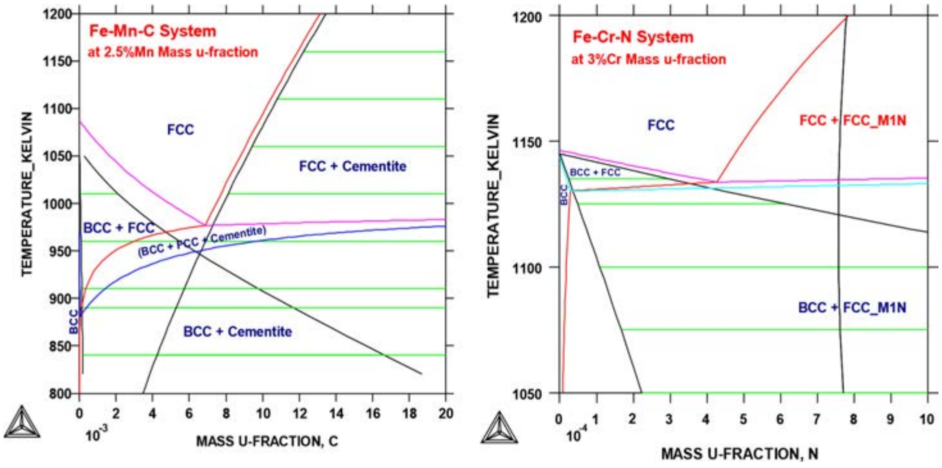
Particularly, there are four issues which you need to consider:

1. Both chosen phases must have similar interstitial/vacancy sub-lattices where the fast-diffusion interstitial component(s) occupy.
2. The choice on the target phase pair must be reasonable for the defined system and specified initial overall composition.
3. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or
4. It is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.

Syntax	step_with_options

	`FAST DIFFUSING COMPONENT: /C/: <INTERSTITIAL COMPONENT(S)>`
	`FAST DIFFUSING COMPONENT: /NONE/: <INTERSTITIAL COMPONENT(S)>`
	The name(s) of the fast-diffusing interstitial component(s) (`C` as the default single component) must be given either one by one at each of the above prompts subsequently or in a combination (separated by an empty space in between, e.g. `C N S`) at the same (first) prompt; otherwise, press <Enter> key to start the paraequilibrium line stepping-calculation.
	Note the following:
	Such specified fast-diffusing interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: These must be located on the interstitial/vacancy sublattices in both chosen phases.
	If there is only one fast-diffusing component which is carbon, press <Enter> to accept the default value (`C`) at the first prompt; if the single fast-diffusing interstitial component is another element (e.g. N), appropriately type interstitial component the name at the first prompt;
	If there are two or more fast-diffusing components (e.g. `C` and `N`), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as `C N`);
	To finish the input of fast-diffusing elements, accept `NONE` at a repeated prompt;
	If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus cancelled entirely.
	During the STEP PARAEQUILIBRIUM calculation procedure, the calculated paraequilibrium states include the:
	• corresponding stepping conditions (e.g. temperature in K, or the stepping composition variable of the matrix component or of one of substitutional components) which has already set as the stepping variable by the SET_AXIS_VAR command);
	• amounts of the phase `A` in mole number [i.e. `NP(phaseA)`];
	• amounts of the phase `B` in mole number [i.e. `NP(phaseB)`];
	• contents of the interstitial component(s) in the phase `A` expressed in u-fractions [i.e. `u-f(phaseA,component(s))`];

Syntax	step_with_options
	- contents of the interstitial component(s) in the phase `B` expressed in u-fractions [i.e. `u-f(phaseB,component(s))`]; - `LNACR(component)` value(s) for the interstitial(s). After a successful STEP PARAEQUILIBRIUM calculation, you can go to the POST module to plot a paraequilibrium phase diagram, or to impose the calculated paraequilibrium states onto a normal phase diagram [normally plotted as a `T-X` isopleth with one of the considered interstitial component(s) as the x-axis variable]. See examples 23 and 42 in the *Console Mode Examples Guide*. However, the stepping calculation procedure for the currently specified paraequilibrium states between the two specified phases may find difficulties at some steps due to some possible numerical problems (normally regarding to the u-fractions of the interstitial components under some composition ranges), or it may completely fails. In the latter case, it implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component(s) and substitutional components. Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.



The figure above shows the plot of a paraequilibrium calculation of isopleths: Formation of para-pearlite in two Fe-based alloys, with equilibrium results appended.

The calculated paraequilibrium phase boundaries (black lines) are shown with tie-lines (in green-colour). In the Fe-2.5Mn-C alloy system, C is considered as fast diffusing interstitial component in the BCC+FCC and FCC+Cementite paraequilibrium stepping calculations; while in the Fe-3Cr-N alloy system, N is treated as fast diffusing interstitial components in the BCC+FCC and FCC+FCC_M1N (i.e. FCC#1+FCC#2) paraequilibrium stepping calculations.

During a STEP calculation, the value of the stepping axis variable for each calculated equilibrium is listed and also the set of stable phases.

You can stop the mapping of a line by pressing a single CTRL-A (under MS Windows) or CTRL-C (under Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by a STEP_WITH_OPTIONS command-sequence, this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30   to hardware
precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value `1.00E-30` to the hardware-dependent precision (under Linux, as `2.00E-14`). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command *SET_NUMERICAL_LIMITS* on page 237 to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Complex miscibility gaps of various solution phases are automatically detected during a stepping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a `Global Test Interval` value and confirming the `Automatically add initial equilibria` in the ADVANCED_OPTION STEP_AND_MAP command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can now start calculating from high temperatures in an austenitic steel (metallic FCC_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC_A1 miscibility-gap, often (while not always) being referred to as `FCC_A1#2, FCC_A1#3`, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC_A1 phase and later also stable.

Occasionally, it may be necessary to have a specified increment other than the default value for the defined stepping axis-variable, in order to calculate/plot a smoother property diagram.

To get a complete property diagram, sometimes (especially in some earlier Thermo-Calc versions) it may also be required to have more than one starting equilibrium-points (under another starting equilibrium condition), and repeat the stepping calculation over the same stepping axis-variable range (while without over-writing the same POLY3 workspaces via a SAVE_WORKSPACE command). However, using the current STEP procedure such a requirement become less necessary.

TABULATE

For any entered table, this command gives a table of values from equilibria calculated with a STEP command. It works only for a table that is entered in either the POLY or POST module.

Unlike the TAB module's command (also called *TABULATE* on page 255) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompts	`NAME: <NAME OF A TABLE ENTERED IN EITHER POLY OR POST>` Specify a table name that is entered in either the POLY or POST module.
	`OUTPOUT ON SCREEN OR FILE /SCREEN/: <FILE NAME OR RETURN>` Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed.

POST Commands

The POST module (post-processor) is available from the POLY module. See *POLY_3 Commands* on page 117 for other information about the POLY module. Read *Using the POST Module* on page 190 before beginning.

In this section:

Using the POST Module

Use the POST module after a *STEP_WITH_OPTIONS* on page 172 or *MAP* on page 158 calculation to generate *graphical* or *tabulated* presentations on screen or into files.

The graphical files are available in different formats (e.g. PS, EMF, PNG, BMP, PDF, JPG, TIF) or data forms (e.g. EXP, TAB and WRL). The graphical output can be phase diagrams, property diagrams, diffusion profiles and other types of plots. The tabulated presentation is into a basic text file (TXT) or a spreadsheet (e.g. an MS Excel file with an extension of .XLS).

The POST module is available through these modules:

- POLY
- TAB
- BIN
- TERN
- POT
- SCHEIL
- POURBAIX

Within the POST module, you can choose any state variable, any derived variable, or any entered symbol (functions or variable) as the X/Y-axis.

Also see *Thermodynamic Variables and Units* on page 271.

When a diagram is plotted, appearance parameters for defining a high-standard graph can be further specified, e.g. curve labelling options, diagram titles and subtitles, plot size, axis length, axis types, axis-tic type, tie-line status, automatic or manual scaling and zooming, semi-automatic or manual labelling on phase boundaries and phase regions, graphic formats, text fonts, colours, raster plot, etc.

You can append experimental data onto a plotted diagram. You can also save the coordinates onto a textual file, which can be edited and used as an experimental data file to be merged onto another diagram or as a part of a setup file for PARROT-module assessment.

Phases can be suspended or restored in a plotted diagram. The reference states for components can also be modified for the resulted diagrams. Moreover, you can translate a plotted property diagram (after a stepping calculation) into a tabulated form, such as a simple list on screen or a textual file, and a spreadsheet .

ADD_LABEL_TEXT

Add a text to an area in a phase diagram or a property diagram. The label is written starting from the specified coordinates. Optionally, you can also let the program automatically add the text by first calculating an equilibrium state at the specified coordinates and then making a label out of the stable phase names.

The label texts and coordinates, either added by this command or modified with *MODIFY_LABEL_TEXT* on page 200 (or manually edited in the **Console Results** window), are stored in the workspace, and these may later be saved onto an *.EXP file (with *MAKE_EXPERIMENTAL_DATAFILE* on page 199).

In some cases such an optional calculation for automatic phase region labelling may not work. It is not possible to automatically add labels for certain sets of axes, like entropy, enthalpy, pH, Eh, etc.

Adding and Editing Plot Labels on page 93 in the *Thermo-Calc User Guide*.

Syntax	ADD_LABEL_TEXT
Prompts	`GIVE X COORDINATE IN AXIS UNITS: <VALUE OF THE X COORDINATE>` Specify the value of the X coordinate where the label is to start.
	`GIVE Y COORDINATE IN AXIS UNITS: <VALUE OF THE X COORDINATE>` The labels disappear if any axis is changed afterwards. Specify the value of the Y coordinate where the label is to start.
	`AUTOMATIC PHASE LABELS? /Y/: <Y OR N>` If you answer Y, the program automatically calculates the equilibrium at the given coordinates and generates a label with the names of the stable phases. However, the automatic calculation works only for phase diagrams that are mapped with two axes in the POLY module, and sometimes it may not work correctly especially for complex heterogeneous interaction systems; in such cases, a message displays.

	`TEXT: <TEXT FOR THE LABEL>`
	If you answer N enter text at the prompt. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.
	LaTeX: You can use LaTeX commands to enter text and symbols. First enter the command followed by the expression or string, for example to display Al2O3 as subscripts:
	`\latex Mole-fraction Al_2O_3`

Syntax	ADD_LABEL_TEXT

	For a list of supported LaTeX commands, see http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html .
	By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.
	To add a mixture of plain text and equation text, you can exit math mode using the string `\textrm` followed by the text to display enclosed in curly brackets. For example `\latex \textrm{Mole-fraction }Al_2O_3` displays this label  $\textrm{Mole-fraction } Al_2O_3$.
	Rotate the text: If you want to rotate the label, start a text string with the rotation command (which is case sensitive and must be in lower case letters) then enter the number of degrees to rotate the label. For example, to rotate the label 45 degrees enter:
	`\rotation 45`
	To rotate the text and use LaTeX, the rotation command must be used first. For example:
	`\rotation 45 \latex Mole-fraction Al_2O_3`
	Rotates the text 45° and includes subscripts in the title Mole-fraction Al2O3.

	`TEXT SIZE: /.35/: <SIZE FOR THE LABEL>` A smaller size of the text may be necessary to fit the label text into the diagram. A default size is given using the latest size in adding label texts, or .35 if the command is called for the first time. A recommended size is e.g. 0.25. These changes to plot labels can also be manually edited in the **Console Results** window.

APPEND_EXPERIMENTAL_DATA

Add experimental data and text onto a calculated diagram. This is done by placing the experimental data and text on a formatted textual file (always having an extension of EXP) that is prepared outside of

Thermo-Calc software (Console Mode and Graphical Mode), according to the syntax of the DATAPLOT Graphical Language.

The picture generated from the data is superimposed on the ordinary graphical output from the postprocessor. Such an experimental data file (*.EXP) may be created by an ordinary textual editor.

Another important usage of this command is to superimpose plots from several independent calculations. For this purpose, there is a command *MAKE_EXPERIMENTAL_DATAFILE* on page 199, which dumps a calculated diagram on an EXP file according to the DATAPLOT syntax. With the aid of a normal text editor, many such files may be merged together. Remember that you can only have one prologue section on each such EXP file.

Also see the *DATPLOT User Guide* included with this documentation set.

Syntax	APPEND_EXPERIMENTAL_DATA
Prompts	`USE EXPERIMENTAL DATA (Y OR N) /N/: <Y OR N>` Specify whether the data from an experimental data file should be included in the next plot. If the answer is `c`, no experimental data are plotted. An **Open** window displays to specify the name of the file with the experimental data.
	`PROLOGUE NUMBER: /0/: <PROLOGUE NUMBER>` Select which prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on. By answering -1, a list of all prologues on the file is given; and by 0, no experimental data are appended.
	`DATASET NUMBER(S) /-1/: <DATASET NUMBER(S)>` Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering -1, a list of all datasets on the file is given; and by 0, no experimental data are appended.

CHANGE_LEGEND

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

LIST_EQUILIBRIUM on page 156 also displays `ORD` (ordered) or `DISORD` (disordered) (when available).

In some cases the legend only shows the phase name for a line when the *SET_LABEL_CURVE_OPTION* on page 209 option is set to `F`.

Syntax	CHANGE_LEGEND
Prompt	`SET SUFFIX FOR PHASE NAMES IN LEGEND? (ALL,NONE,CONSTITUTION,ORDERING) /NONE/:` When you select `None` the legend includes the standard information about the phases. When you select `All` the Constitution description and the Ordering description (when there is ordering) are also included. When you select `Constitution`, this is added to the standard description. When you select `Ordering` and when there is ordering, this is added to the standard description.
	Also see *About Legend Styles* on page 92 in the *Thermo-Calc User Guide* for examples of these labels.

DUMP_DIAGRAM

After a Thermo-Calc graph is created (and displays with the PLOT_DIAGRAM command) you can save (dump) a diagram to a file so you can quickly print it. It is similar to the PRINT_DIAGRAM command.

Similar to *PRINT_DIAGRAM* on page 201, it does not matter what graphic device is set up for the graph, this command is always able to convert the graph shown on screen to the selected graphic format.

Syntax	DUMP_DIAGRAM
Prompt	`OUTPUT FORMAT /: <FORMAT OR RETURN>` Specify an appropriate graphic format for dumping the graph or pressing <Enter> to accept the default format.
	A **Save** window opens if you have not specified a filename. Select a directory path and enter a **File name**. If a file with the specified name already exists, then you are prompted whether to overwrite the old file or not. The third argument of the command allows you to specify whether to overwrite (`Y`) the old file or not (`N`).

After the printing process is finished, the temporarily set graphic device for conversion and printing is switched back to the one set by the command *SET_PLOT_FORMAT* on page 210, so that you can save the graph in file(s) using *PLOT_DIAGRAM* on page 200.

ENTER_SYMBOL

The information about this command is specific to the Thermo-Calc POST and POLY modules in Console Mode.

Symbols are a useful feature of the POLY and POST modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C_E command), stepping calculation (enforced by the command *STEP_WITH_OPTIONS* on page 172) or mapping calculation (enforced by *MAP* on page 158). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using *EVALUATE_FUNCTIONS* on page 155 before showing the corresponding values in the calculated equilibrium state.

The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.

Also see *ENTER_SYMBOL* on page 72 for the GIBBS Module.

See example 44 in the *Console Mode Examples Guide*for an example of using variables and functions.

Syntax	ENTER_SYMBOL
Prompt	`CONSTANT, VARIABLE, FUNCTION OR TABLE? /FUNCTION/: <KEYWORD>` The `Keyword` can be specified as `CONSTANT`, `VARIABLE`, `FUNCTION` or `TABLE`. • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by `P0` after the command ENTER CONSTANT `P0=101325`. Defined constants can be used as values in condition assignments, for example, `SET-COND P=P0`. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an *EVALUATE_FUNCTIONS* on page 155 command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET-CONDITION command. • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST. There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.
	`NAME: <NAME OF THE SYMBOL>` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names. You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, `TC=T-273.15` or `T_C=T273.15` which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.

Syntax	ENTER_SYMBOL

For different types of symbol (constant, function, variable or table), the questions have different prompts.

`FUNCTION: <DEFINITION FOR A FUNCTION OR VARIABLE>`

Functions and *variables* are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).

Unary functions like `LOG`, `LOG10`, `EXP`, `SIN`, `COS` and `ERF` can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing <Enter> at the next prompt).

Examples of function expressions:

- `GM(LIQUID)`: The Gibbs energy of liquid per mole component
- `H.T/4.184`: The heat capacity of the system in calories
- `ACR(CR)/X(FCC,CR)`: The activity coefficient for Cr in FCC
- `T-273.15`: The temperature in Celsius

`&: <CONTINUATION OF THE DEFINITION FOR THE SYMBOL>`

The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.

`VALUE: <VALUE FOR A CONSTANT>`

A *constant* can only be assigned a numeric value once.

`VALUE OR EXPRESSION: <VALUE OF EXPRESSION FOR A VARIABLE>`

A *variable* can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.

`VARIABLE(S): <VARIABLE(S) IN A TABLE>`

A *table* consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.

Example:

```
ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)
```

Which means that the table called K contains four columns, i.e. the temperature, the mole

Syntax	ENTER_SYMBOL
	fractions of C and Cr in the LIQUID phase, and the activity of C. To show the temperature in Celsius in a table, give the command ENTER FUNCTION `TC=T-273;` and then use the symbol `TC` in the table. `& <CONTINUATION OF THE DEFINITION FOR THE TABLE>` The ampersand `&` means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press <Enter> again.

FIND_LINE

Identifies various property curves on a plotted property diagram (after a stepping calculation); it also works well in find stable phase regions on a phase diagram (after a mapping calculation).

Syntax	FIND_LINE
Prompts	`X COORDINATE /.484623611/: <VALUE OF THE X COORDINATE>` Specify the `value of the X coordinate` where you want to find the details of property curve (or phase region).
	`Y COORDINATE /.5153737962/: <VALUE OF THE Y COORDINATE>` Specify the `value of the Y coordinate` where you want to find the details of property curve (or phase region). The POST module displays the identified property (for a property curve on a property diagram), or the identified stable phase-assemblage (for a phase region on a phase diagram).

LIST_DATA_TABLE

This command is used for listing various properties (i.e. the Y-axis variable on a property diagram) that change with an independent variable (i.e. the X-axis variable on a property diagram), which have already been defined in the POST module (and often are plotted on the **Console Results** window), but only after a STEP calculation.

The listing output can be either on screen or in a spreadsheet file in the MS Excel format (under specified file name with the default file extension of XLS), which can be further edited or used for graphical handling by opening the file (using the MS-Excel program) outside of the Thermo-Calc software system.

Syntax	LIST_DATA_TABLE
Prompt	`OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME OR RETURN >` Specify a file name if you want to save on a spreadsheet file (in the MS Excel format, with the default extension of `XLS`) on which the already-defined properties on a property diagram (after a STEP calculation) is saved, or press <Enter> if want to see a simple textual table on screen (for the already-defined properties that change alone with an independent variable). This command only works for a property diagram after a stepping calculation but not for any phase diagram after a mapping calculation.

LIST_PLOT_SETTINGS

Syntax	LIST_PLOT_SETTINGS
	Lists the present values of most parameters specifying the type of diagram to be plotted.

LIST_SYMBOLS

For both the POLY and POST modules, list the definitions for all constants, functions, variables and tables.

In order to find the value of a function or variable, use *SHOW_VALUE* on page 172 or *EVALUATE_FUNCTIONS* on page 155. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %.

MAKE_EXPERIMENTAL_DATAFILE

Write the graphical information onto screen or a formatted text file (always having an extension of EXP) using the DATAPLOT graphical format. In order to merge two or more diagrams from separate calculations, you can write them out on files with this command, and then add/edit them together with a normal textual editor.

Also see the *DATPLOT User Guide* included with this documentation set.

Syntax	MAKE_EXPERIMENTAL_DATAFILE
Prompt	`OUTPUT TO SCREEN OR FILE /SCREEN/: <NAME OF A FILE OR RETURN>` Specify the name of the desired file. Accept `SCREEN` (press <Enter>) for a list Otherwise, a file name where the graphical information is written must be given here. The default file extension is EXP (under MS Windows) or exp (under Linux).

MODIFY_LABEL_TEXT

Move a label created with the command *ADD_LABEL_TEXT* on page 190 to another position, or replace its text with another one.

The label texts and the coordinates, either added by ADD_LABEL_TEXT command or modified by this command or manually edited on the Console Results window, are stored in the workspace, and can be saved onto an *.EXP file (through *MAKE_EXPERIMENTAL_DATAFILE* on the previous page).

Syntax	MODIFY_LABEL_TEXT
Prompts	`WHICH LABEL TO MODIFY? /#/: <NUMBER OF THE LABEL>` Before this prompt, all the labels created by the ADD_LABEL_TEXT command is listed with an identifying number. Specify the `number of the label` you want to modify. The default one (#) is the last added label.
	`NEW X COORDINATE: /XXX/: <NEW X POSITION>` Specify the `new X position`. The previous X coordinate is displayed. Press <Enter> to accept.
	`NEW Y COORDINATE: /YYY/: <NEW Y POSITION>` Specify the `new Y position`. The previous Y coordinate is displayed. Press <Enter> to accept.
	`NEW TEXT /ABCDEFGH.../: <NEW LABELING TEXT>` Specify the `new labeling text`. The previous text is displayed. Press <Enter> to accept. ⓘ The new label text must not be longer than the previous text.

PLOT_DIAGRAM

With this command, a calculated/plotted diagram is displayed if the default graphic device has already been defined by the *SET_PLOT_FORMAT* on page 210 command. It can also be saved onto a file.

The diagram axes must be set first.

The functionality of this command is shared in two ways:

- in PLOT_DIAGRAM for normal screen display and file saving and
- in *PRINT_DIAGRAM* below (under MS-Windows environment) for direct hard-copy printing.

Syntax	PLOT_DIAGRAM
Prompt	`OUTPUT TO SCREEN OR FILE /SCREEN/: <NAME OF A FILE OR RETURN FOR SCREEN>`
	Specify the name of the desired file (Note that under Linux, the prompt is `PLOTFILE /SCREEN/`). Consequently, a file with a proper extension for the selected graphic format (set by the SET_PLOT_FORMAT command) is saved under the current working directory. If no extension is given in the file name, the default extension e.g. ps for Postscript portrait/landscape modes, P7 or p7 for HPGL landscape, P8 or p8 for HPGL portrait, etc.) is automatically given to the file name. If the default device is set (by the command SET_PLOT_FORMAT), you can either accept `SCREEN` to plot the graph in the Thermo-Calc Graph window on screen by pressing <Enter>, or save it on a file by giving a file name.

PRINT_DIAGRAM

Syntax	PRINT_DIAGRAM
	Print with high quality to a file after a Thermo-Calc graph is created (and is displayed with *PLOT_DIAGRAM* on the previous page). It has the same function as the Print Plot option on the Console Results windows.

QUICK_EXPERIMENTAL_PLOT

This is similar to *APPEND_EXPERIMENTAL_DATA* on page 192 but can be used when there is no graphical information to be plotted in the POLY3 workspace. It defines a pair of axis, sets the axis labels to X and Y, and scales both X- and Y-axes between 0.0 and 1.0 unless a prologue is read from the DATAPLOT (*.EXP) data file.

Also see the *DATPLOT User Guide* included with this documentation set.

Syntax	QUICK_EXPERIMENTAL_PLOT
Prompts	`PROLOGUE NUMBER: /0/: <PROLOGUE NUMBER>` An **Open** window displays. Select the prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on. By answering -1, a list of all prologues on the file is given; and with 0, no experimental data are appended.
	`DATASET NUMBER(S) /-1/: <DATASET NUMBER(S)>` Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering `-1`, a list of all datasets on the file is given; and with `0`, no experimental data are appended.

REINITIATE_PLOT_SETTINGS

All parameters describing the diagram are given default values.

Syntax	REINITIATE_PLOT_SETTINGS
	All plot settings made in the POST module are deleted, and it returns to the initial settings when the POST module is entered.

RESTORE_PHASE_IN_PLOT

Restores a phase previously suspended from the plot with *SUSPEND_PHASE_IN_PLOT* on page 216. It works only after at least one phase is suspended.

Syntax	RESTORE_PHASE_IN_PLOT
Prompt	`PHASE NAME: <NAME OF A PHASE>` Give the name of the phase to be restored.

SELECT_PLOT

Select a plot within the current Results tab in the Console Results window.

Syntax	SELECT_PLOT
Prompt	`PLOT <N/NEW>` Where `N` is a positive integer. Enter the number of the plot that is selected in the **Console Results** window (in the currently selected **Results** tab). If a plot with that number does not exist, it is created. The default parameter value is `NEW`. If this is entered, then a new plot is created. Create a new plot can also be done by pressing Ctrl+Shift+T.

SET_AXIS_LENGTH

Change the real length of an axis in inches. The default number of tic-marks on an axis is 10 when the relative length is 1. The number and units per tic-mark must be a multiple of 1, 2 or 5 to obtain a reasonable scaling of an axis.

Syntax	SET_AXIS_LENGTH
Prompts	`AXIS (X, Y OR Z): <NAME OF AN AXIS>` Specify which axis to set the length.
	`AXIS LENGTH /11.5/: <NEW RELATIVE AXIS LENGTH>` Specify the new real axis length in inches. The relative length 1 corresponds to 10 tic-marks on the axis.

SET_AXIS_PLOT_STATUS

Specify whether the axis title texts and axis label texts are to be plotted or not on a diagram. It does not work for the axis lines and tic-marks. If you want to plot a diagram without tic-marks, use *SET_TIC_TYPE* on page 215 first.

This can be used to merge different diagrams on a pen-plotter or to obtain the diagram faster. The default status is that all the set axes are to be plotted.

Syntax	SET_AXIS_PLOT_STATUS
Prompt	`AXIS PLOT (Y OR N) /Y/: (Y OR N)` Specify to plot axis texts (`Y`) or no (`N`).

SET_AXIS_TEXT_STATUS

Change the axis text from the automatic text given by the axis specification to a text.

Syntax	SET_AXIS_TEXT_STATUS
Prompts	`AXIS (X, Y OR Z): <NAME OF AN AXIS>` Specify which axis text status to change.
	`AUTOMATIC AXIS TEXT (Y OR N) /N/: <Y OR N>` Specify if automatic axis text is to be used (`Y`) or (`N`). If you answer `N`, enter axis text.
	`AXIS TEXT: <ENTER AXIS TEXT>` You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.

Syntax	SET_AXIS_TEXT_STATUS
	Also see *ADD_LABEL_TEXT* on page 190.

SET_AXIS_TYPE

Change the axis type among linear, logarithmic and inverse axis.

Syntax	SET_AXIS_TYPE
Prompts	`AXIS (X, Y OR Z): <NAME OF AN AXIS>` Specify which axis to change the axis type.
	`AXIS TYPE /LINEAR/: <NEW AXIS TYPE>` Specify which new axis type to set. Select `LIN`ear (default), `LOG`arithmic or `INV`erse. Only the three first characters are relevant.

SET_COLOR

Some devices support colours or line thickness. With this command, select different colors or line types on some types of information on a diagram.

This command can fail if a chosen device does not support colors or line thickness.

This command gives four sequential prompts (i.e. Text and axis, Invariant equilibria, Tie-lines, and All other lines), with the Keyword and default option (both listed below). Depending on if the switched-on graphic device (by the SET_PLOT_FORMAT command) supports colors or line types, the POST automatically switches on the appropriate Keyword.

Syntax	SET_COLOR

Prompt	`TEXT AND AXIS KEYWORD /DEFAULT OPTION/`
	`<RETURN OR NEW OPTION>`
	`INVARIANT EQUILIBRIA KEYWORD /DEFAULT OPTION/: <RETURN OR NEW OPTION>`
	`TIE-LINES COLOR KEYWORD /DEFAULT OPTION/: <RETURN OR NEW OPTION>`
	`KEYWORD OF ALL OTHER LINES /DEFAULT OPTION/: <RETURN OR NEW OPTION>`
	This is usually for the solubility lines.

Syntax	SET_COLOR
	☑ The `Keyword` is either `Color` or `LineType`, depending on if color or line type is supported by the switched-on graphic device (by the *SET_PLOT_FORMAT* on page 210 command); the POST module *automatically* switches on the appropriate `Keyword`.

Color Options

The options for `Color` are:

BACKGROUND	BLUE	PURPLE	GRAY
FOREGROUND (default)	YELLOW	GOLD4	ORANGERED3
RED (default for invariant equilibria)	MAGENTA	TURQUOISE4	MAROON
GREEN (default for tie lines)	CYAN	PINK	PLUM
	SIENNA	OLIVEDRAB	SEAGREEN
	ORANGE1	CORAL1	USERDEF

LineType Options

The options for `LineType` are:

INVISIBLE	VERY_THICK (default for invariant equilibria)
NORMAL (default)	THIN (default for tie lines)
THICK	VERY_THIN
DASHED	DOTTED

SET_CORNER_TEXT

Adds text to the corners on a plotted diagram. Normally, you can write such texts as a subtitle.

The primary database (not the appended ones) used in calculations and the calculated conditions are automatically plotted at the upper-left corner as a part of the header on all plotted diagram. Unless the plotting option WRITE CONDITIONS is switched off by the command *SET_PLOT_OPTIONS* on page 211, the calculated conditions are always written on plotted diagrams; and only when the plotting option PLOT HEADER is switched off by the command SET_PLOT_OPTION, the used database also always appear. Under such circumstance, avoid writing texts at the UPPER_LEFT corners.

Syntax	SET_CORNER_TEXT
Prompt	`CORNER /LOWER_LEFT/: <RETURN OR NEW OPTION>` Choose an option: • LOWER_LEFT • UPPER_LEFT • UPPER_RIGHT • LOWER_RIGHT • TOP_OF_TRIANGLE
	`TEXT: <TEXTS AS A SUBTITLE OR A NOTE>` Write the texts that are to be written on the specified diagram corner.

SET_DIAGRAM_AXIS

Specify an axis variable for a plot or a listing. To be able to plot a diagram, at least two axis variables (`X` and `Y`) must be specified. In the Thermo-Calc Console Mode, three axes (`X`, `Y` and `Z`) can be specified for a diagram.

The axis variables in the plot can be different from the number of axis used for the mapping.

If you want to plot a phase diagram with tie-lines in the plane after a MAP calculation, then the composition axis must be `mole-fraction` or `weight-fraction`, or `mole-percent` or `weight-percent` of one specific component. You must not use the stable variable `x(comp)` or `w(comp)` even if that is what you used when calculating the diagram, because that only gives one side of the two-phase region. It may be sufficient to indicate that mole-fraction is the same as the stable variable `x(*,comp)`, and weight-fraction is the same as the stable variable `w(*,comp)`.

If you plot a phase diagram where the tie-lines are not in the plane after a MAP calculation, then `mole-fraction` and `x(comp)` are identical.

When you plot a property diagram after a STEP calculation and want a composition axis variable, you should normally use x(comp) and not mole-fraction.

The axis must have exactly the same number of columns, or one axis must have one column. In the first case the columns are plotted matching them one by one; in the latter all columns on one axis is plotted against the single column. For example, you can have the temperature on one axis and the amount of each phase on the other. The amount of each phase is the state variable `NP(*)` in mole fraction or `BPW(*)` for mass fractions of phases.

Automatic diagram axis: The POST module can set automatic diagram axis identical to those used in the *MAP* on page 158 command.

If the state variable `x(comp)` is used in a MAP calculation, then mole-fraction of the component is used as diagram axis; if a potential or some other state variables are used, then that is used as a diagram axis.

After a STEP calculation, automatic diagram axis is not set as there is only one axis used in the calculation.

Syntax	SET_DIAGRAM_AXIS
	`AXIS (X, Y OR Z): <AXIS NAME>` Specify which axis (X or Y or Z) to set with a variable.
Prompts	`VARIABLE TYPE: <VARIABLE NAME>` Specify a variable for the chosen axis here. The valid variables are: • TEMPERATURE-CELSIUS as temperature in oC • TEMPERATURE as temperature in K • PRESSURE as pressure in Pa • ACTIVITY for a component • LNACTIVITY for a component [ln(ACR(component)] • MOLE-FRACTION for a component • MOLE-PERCENT for a component • WEIGHT-FRACTION for a component • WEIGHT-PERCENT for a component • NONE to clear the axis • Any valid state variable including those with wildcards, e.g. NP(*) or x (*,component). Due to the use of wildcard * in such a state variable, the program asks for a column number. • Any entered function or variable. • Any entered table.
	If you specify an entered table as the variable, then you are given these prompts: `FOR COMPONENT: <COMPONENT NAME>`

Syntax	SET_DIAGRAM_AXIS
	When an activity, mole or weight fraction or percent of a component shall be plotted, the component name must be supplied here.
	`COLUMN NUMBER: <COLUMN NUMBER(S)>` Specify the column number(s) in the chosen table that are to be plotted onto the earlier specified axis. For example: • `1` for column 1 • `2,3` for columns 2 and 3 • `2,3 >5` for column 2,3 and all columns above column 5 • * for all columns

SET_DIAGRAM_TYPE

Choose the diagram type as perpendicular plot or triangular plot (Gibbs triangle, especially for ternary systems). The default is with a perpendicular axes.

For phase diagrams of ternary or pseudo-ternary systems, it is usually need to plot isothermal sections as triangular grams. If desired, all lines outside the region limited by a line joining the end points of the X- and Y-axis is removed.

In order to create a 3D-plot file (in the VRML format, *.WRL) for a tetrahedron diagram, this command in the sequence SET_DIAGRAM_TYPE N Y should be used first.

Syntax	SET_DIAGRAM_TYPE
Prompts	`TRIANGULAR DIAGRAM (Y OR N) /N/: <Y OR N>` Specify a triangular plot `Y`. Otherwise (by pressing <Enter> to accept `N`), perpendicular axis is set and this command is terminated. By default, perpendicular diagrams have (almost) the same scaling on both axes.
	`CREATE TETRAHEDRON WRML FILE (Y OR N) /N/: <Y OR N>` If a triangular plot is not selected (at the above prompt), answer `Y` in case a tetrahedron diagram is used to generate VRML (`*.WRL`) file by sequentially using the CREATE_3D_PLOTFILE command.
	`PLOT 3:RD AXIS (Y OR N) /N/: <Y OR N>` If a triangular plot is selected, specify if a 3rd axis (by answering Y here), connecting the end points of the X- and Y-axes, is plotted.

Syntax	SET_DIAGRAM_TYPE
	`CLIP ALONG 3:RD AXIS (Y OR N) /N/: <Y OR N>` If a triangular plot is selected, all lines outside the region limited by a line joining the end points of the X- and Y-axis are removed by answering Yes (`Y`).

SET_FONT

Select the font to use for labels and numbers when plotting the diagram under the currently selected graphic device (*SET_PLOT_FORMAT* on the next page). For some devices there may be other fonts available and these are selected by the SET_PLOT_FORMAT command.

Syntax	SET_FONT
Prompts	`SELECT FONTNUMBER /1/: <#>` Specify an available font number # as the default font for the current graphic device, or accept the font number 1 by pressing <Enter>. By typing a question mark ? here, the program lists the available fonts under the currently selected graphic device.
	`FONT SIZE /.34/: <##>` The size of the chosen font is specified. A value around 0.34 is recommended.

SET_INTERACTIVE_MODE

Syntax	SET_INTERACTIVE_MODE
	Resets the input and output units to their initial values, i.e. keyboard and screen. Remember to add this as the last command to your MACRO files, in order to stop execution of the command file in the POST module. It has no meaning in interactive mode.

SET_LABEL_CURVE_OPTION

Identify the curves drawn in the post-processor by marking each curve with a digit and then list the meaning of these digits beside the plot.

The number of digits can be quite large in some cases. If so, use the SET_FONT command and reduce the font size; usually, 0.2 is sufficient.

Syntax	SET_LABEL_CURVE_OPTION
Prompt	`CURVE LABEL OPTION (A, B, C, D, E, F OR N) /A/: <OPTION>`

The options:

- `A`: List stable phases along line
- `B`: As A but curves with same fix phase have same number
- `C`: List axis quantities
- `D`: As `C` but curves with same quantities have same number
- `E`: As `B` with changing colors
- `F`: As `D` with changing colors
- `N`: No labels

This question is rather cryptic but usually the option B or E is good for phase diagrams (after a MAP command) and option D or F for property diagrams (after a STEP command). Those interested can try out the option A and C by themselves.

Option B or E lists the fixed phases along each curve, whereas option D or F gives the axis variables used along each curve. E provides varied colors for different stable-phase curves on phase diagrams (after a MAP command); F provides varied colors for different property curves on property diagrams (after a STEP command). The option `N` (NONE) disables all curve labels and lists.

If, for example, you use `T` (temperature in K) as the variable axis in a STEP command and then plot the amount of stable phases (with *SET_DIAGRAM_AXIS* on page 206 `Y NP(*)`) on the Y-axis versus `T-C` on the X-axis, then the list may have lines like:

```
1: T-273.15, NP(LIQUID)
2: T-273.15, NP(FCC_A1)
```

This means that for curve `1` the X-axis is `T-273.15` (the same for all curves, of course) and `NP(LIQUID)` on the Y-axis. Curve `2` has the same X-axis but `NP(FCC_A1)` on the Y-axis.

SET_PLOT_FORMAT

Set the format of the graphical output to different graphical devices. The default graphic device is normally for screen output (number 22 - TCUNITE Driver). Legacy devices can still be used (1 for Windows and 9 for XWindow for Linux). This default graphic device value may also be altered with *SET_PLOT_ENVIRONMENT* on page 245 in the system monitor or by your TC.INI file.

Syntax	SET_PLOT_FORMAT
Prompt	`GRAPHIC DEVICE NUMBER /#/: <NUMBER OF THE DEVICE>` Specify a graphic device number. Depending on the hardware, different plot formats (graphic devices) may be available. These are listed online by giving a question mark ?. For some formats there can be additional sub-prompts, asking for if using (YES) or not using (NO) the fonts available for the chosen format, and if YES for further specifications, e.g. font type and size.

SET_PLOT_OPTIONS

You are prompted for and can toggle on (`Y`) or off (`N`) the plotting of some options on all subsequently generated diagrams.

For the `Always initiate POST on re-entering` prompt, the default is Y which implies that the POST module automatically reinitiates whenever the POLY3 workspace is changed upon re-entering. If answered N the same diagram axis variables are kept even if the workspaces in the POLY module are read from or written to an *.POLY3 file. The N answer is useful when there are several sets of *.POLY3 files with the same calculation but for different sets of model parameters.

For the `Always solid line` prompt, the default answer is `N` which means that the POST module plots solid lines for stable phases but dashed lines for metastable phases. This is normally for plotting property diagram after a STEPPING calculation; however, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. When the alternative answer Y is chosen, all the lines are always plotted in solid lines.

Syntax	SET_PLOT_OPTIONS
Prompts	`PLOT HEADER /Y/: <Y OR N>` Toggle the plotting of the Thermo-Calc header text above a diagram.
	`PLOT LOGO /Y/: <Y OR N>` Toggle the plotting of the Thermo-Calc logotype at the lower-left corner of a diagram.
	`PLOT FOOTER /Y/: <Y OR N>` Toggle the plotting of the footer identifier text at the right margin of a diagram.
	`WHITE-CONTOURED-PS-CHARS /Y/: <Y OR N>` This makes it possible to write PostScript characters in white contoured status.
	`PLOT REMOTE EXPONENT(S) /Y/: <Y OR N>`

Syntax	SET_PLOT_OPTIONS
	This sets (`Y`) or removes (`N`) the plotting of the remote exponent on the axis.
	`PLOT SYMBOLS AT NODE POINTS /0/: <#>` This makes it possible to plot symbols at the node points on plotted lines on a diagram.
	`SYMBOL SIZE /.1/: <.#>` Set the size of symbols which are plotted at the node points.
	`WRITE CONDITION? /Y/: <Y OR N>` The initial equilibrium conditions for the current calculations are automatically plotted at the upper-left corner as a part of the header. With this option switched off (by answering `N`), it makes possible to not write the calculated conditions on a plotted diagram.
	`WRITE DATABASE NAME? /Y/: <Y OR N>` Primary database (not the appended ones) used in the current calculations are automatically plotted at the upper-left corner as a part of the header. With this option switched off (by answering `N`), it makes possible to not write the database name on a plotted diagram.
	`ALWAYS INITIATE POST ON RE-ENTERING: /Y/: <Y OR N>` `Y` lets the POST module automatically reinitiate whenever the POLY3 workspaces are changed upon re-entering. If answered `N`, the same diagram axis variables are kept even if the workspaces in the POLY module is read from or written to an *.POLY3 file. Answering `N` is useful when there are several sets of *.POLY3 files with the same calculation but for different set of model parameters.
	`ALWAYS SOLID LINE: /N/: <Y OR N>` `N` allows the POST module to plot solid lines for stable phases but dashed lines for metastable phases. This is normally for plotting property diagram after a STEPPING calculation; however, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. When answered `Y` all the lines are always plotted in solid lines.

SET_PLOT_SIZE

Change the size of the diagram by specifying a global plot size (as a relative scaling factor). The default value of the relative scaling factor is 1, while the real size of the plotted diagram depends on what output device is chosen with *SET_PLOT_FORMAT* on page 210. The default plot size (corresponding to the default global plot size 1) is adjusted to the chosen device.

Syntax	SET_PLOT_SIZE
Prompt	`GLOBAL PLOT SIZE /1/: <RELATIVE SCALING FACTOR>` Enter the relative scaling factor as a numerical number (e.g. `0.5`, `0.8`, `1.0`, `1.5`, etc.). By pressing <Enter>, the default relative scaling factor (`1`) is accepted.

SET_PREFIX_SCALING

Set the prefix scaling of remote exponents with certain powers (default is 3), by taking as argument with an `axis name` and a `YES`, or `NO`, or an integer number # (as the powers for the remote exponents):

`NO` switches off its action.

`YES` arranges the prefix scaling so that the axis scaling is done with the remote exponents being powers of three, i.e. `...,-6,-3,0,3,6,...`

sets the remote exponents as being powers of #.

Syntax	SET_PREFIX_SCALING
Prompt	`AXIS (X, Y OR Z): <NAME OF AN AXIS>` Specify which axis is to have a prefix scaling.
	`USE PREFIX SCALING /Y/: (Y OR N OR #)` Answer either `Y` or `N` or an integer number as described above.

SET_RASTER_STATUS

Plot a raster (i.e. with gridlines on both axis directions) in the diagram. The default status is no raster plotted.

Syntax	SET_RASTER_STATUS
Prompt	`RASTER PLOT (Y OR N) /N/: <Y OR N>` Enable (Y) or disable (N) the raster plot.

SET_REFERENCE_STATE

The reference state for a component is important when calculating activities, chemical potentials and enthalpies. After calculating with *STEP_WITH_OPTIONS* on page 172 or *MAP* on page 158, the reference state for a component can also be changed for plotting various properties of the component in the entire system or in a specific phase by using this command. Afterwards, you can set diagram axes as chemical potential or activity quantities with the R suffix, i.e. MUR(comp), MUR(comp,ph), ACR(comp), ACR (comp,ph) or their common logarithms [e.g. LNACR(comp,ph)].

Syntax	SET_REFERENCE_STATE
Prompts	`COMPONENT: <NAME OF THE COMPONENT>` The name of the component must be given.
	`REFERENCE STATE: <NAME OF A PHASE USED AS THE NEW REFERENCE STATE>` The `Name of a phase`, that must be either ENTERED, DORMANT or SUSPENDED, is given here. The component must, of course, be a constituent of this phase. A subtle problem is that if the component exists in several species in the phase, for example, oxygen as O, O2 and O3 in a gas. Normally, you would like to have the most stable species as reference state of oxygen, i.e. O2 in this case. When setting the reference state, a one-time calculation is made for the Gibbs energy. This is for all possible states with the pure component phase at the current temperature and the command selects the most stable one as the reference state.
	`TEMPERATURE /*/: <REFERENCE TEMPERATURE>` Select the temperature (in K) for the reference state. The value * means the current temperature is used for the calculation.
	`PRESSURE /1E5/: <REFERENCE PRESSURE>` Select the pressure (in Pa) for the reference state. The value * means the current pressure is used for the calculation.

SET_SCALING_STATUS

When an axis variable is selected by *SET_DIAGRAM_AXIS* on page 206, the scaling status for the axis is always set to automatic scaling. By this command, choose between manual or automatic scaling on a specified axis. If manual scaling is chosen, specify a minimum and a maximum value. Manual scaling can be used to magnify interesting parts of a diagram.

Syntax	SET_SCALING_STATUS
Prompts	`AXIS (X, Y OR Z): <NAME OF AN AXIS>` Specify which axis that you want to set the scaling status.
	`AUTOMATIC SCALING (Y OR N) /N/: <Y OR N>` Choose between automatic (Y) and manual scaling (N). For manual scaling specify these parameters:
	`MIN VALUE: <MINIMUM VALUE>` The minimum value at the start point of the specified axis.
	`MAX VALUE: <MAXIMUM VALUE>`

Syntax	SET_SCALING_STATUS
	The maximum value at the end point of the specified axis.

SET_TIC_TYPE

Change the drawing of the axis tics. You may alter the placement of tic marks on the axis, e.g. inside or outside or no tic marks. The size of tic marks cannot be altered by this command, but these are adjusted based on the selected graphic device and the defined relative scaling factor (global plot size).

Syntax	SET_TIC_TYPE
Prompt	`TIC TYPE /1/: <1 OR -1 OR 0>` The tic type 1 is default, i.e. the tics are drawn outside the diagram. -1 means that the tics are inside the diagram and 0 means no tics.

SET_TIELINE_STATUS

If the tie-lines are in the plane of the calculation, you can select to plot the tie-lines in two-phase fields with this command.

Syntax	SET_TIELINE_STATUS
Prompt	`PLOTTING EVERY TIE-LINE NO /0/: <NUMBER OF TIE-LINES>` The tie-lines plotted are not equally spaced by the graphics software. Instead, you can select to plot a subset of the calculated tie-lines, i.e. every one (1), every second (2), every three (3), etc. By accepting the default value 0, no tie-line is plotted.

SET_TITLE

Specify a title that displays on all listed tables and plotted diagrams from the POST module in the same run of Console Mode.

Syntax	SET_TITLE
Prompt	`TITLE: <TITLE>` Enter the title you want to appear on all tabulation or graphic outputs. ✎ There is a maximum length of about 60 characters for the title. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.
	➲ Also see *ADD_LABEL_TEXT* on page 190.

SET_TRUE_MANUAL_SCALING

The tic-marks on the axes are normally placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this. If such an automatic adjustment behaviour is unwanted, it can be avoided by using this command (followed by a message showing the TRUE MANUAL SCALING set for a specific axis).

The command works like a toggle. To reset the automatic scaling behaviour, repeat the command a second time for that specific axis (followed by a message saying the SEMI_MANUAL SCALING set for the specific axis.

Syntax	SET_TRUE_MANUAL_SCALING
Prompt	`AXIS (X, Y OR Z): <NAME OF AN AXIS>` Specify which axis (X or Y or Z) you want to toggle between automatic adjustments or avoid the adjustment of the given maximum and minimum values.

SUSPEND_PHASE_IN_PLOT

Specify that lines originating from the presence of a certain phase shall not be plotted on a diagram. If you want to bring the suspended phase back to the diagram, use *RESTORE_PHASE_IN_PLOT* on page 202.

Syntax	SUSPEND_PHASE_IN_PLOT
Prompt	`PHASE NAME: <NAME OF A PHASE>` Specify the name of the phase to be suspended from the diagram.

TABULATE

For any entered table, this command gives a table of values from equilibria calculated with a STEP command. It works only for a table that is entered in either the POLY or POST module.

Unlike the TAB module's command (also called *TABULATE* on page 255) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompts	`NAME: <NAME OF A TABLE ENTERED IN EITHER POLY OR POST>` Specify a table name that is entered in either the POLY or POST module.
	`OUTPOUT ON SCREEN OR FILE /SCREEN/: <FILE NAME OR RETURN>` Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed.

POTENTIAL_DIAGRAM Module

In this section:

POTENTIAL_DIAGRAM

The POTENTIAL_DIAGRAM module (short name, the POTENTIAL module) is a potential phase diagram calculation module.

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

To enter the module, at the SYS prompt type `GOTO_MODULE POTENTIAL`.

There are no commands for this module. Follow the prompts and see *About Potential Diagrams* on page 160 in the *Thermo-Calc User Guide* for details about how to calculate using potential diagrams.

See example 35 in the *Console Mode Examples Guide*.

Syntax	POTENTIAL_DIAGRAM
Prompts	`DATABASE: /POT/` Press <Enter> and the program lists the available databases. Type one of the database names and press <Enter> to select. The following default elements are then based on the chosen database.
	`MATRIX ELEMENT: /FE/`
	`FIRST POTENTIAL SPECIES: /S1O2/`
	`SECOND POTENTIAL SPECIES: /O2/`
	`TEMPERATURE: /1000/`

POURBAIX_DIAGRAM Commands

Also search the online help or see the Pourbaix diagrams educational material and the *Thermo-Calc User Guide*.

In this section:

POURBAIX_DIAGRAM Commands

Also search the online help for additional information in other guides.

See examples TCEX40 and TCEX53 in the *Console Mode Examples Guide*.

After you enter the POURBAIX_DIAGRAM module, you are prompted with the following:

```
NEED ANY INSTRUCTION ON THE POURBAIX MODULE? /N/:Y
```

If you answer `Y` the following notes are displayed.

- The Pourbaix diagram is actually a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (Eh, as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modelled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).
- At least one database is required that contains an AQUEOUS solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc database spectrum, or be chosen from an appropriate USER-specified database (it must be in the Thermo-Calc TDB format).
- Due to the restrictions of aqueous solution model used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ) or AQS (PAQS) for AQUEOUS solution phase. Among others, one should keep in mind the following regulations:
  - The ELECTRON is defined as an special element (ZE) and as the only constituent in its reference phase REFERENCE_ELECTRODE (for determining the electropotential that is defined as Eh with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;
  - The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;

- The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.

- Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H2O1, O2 and H2; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!
- All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a GASeous mixture phase, a REF_ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above).

Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the TCAQ or AQS as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended). Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAl, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for GASeous mixture phase and for varous solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.

- The current advanced POURBAIX-Module has been designed and developed in an efficient and effective way that it only requires the user to just answer some simple and necessary questions, rather than to go through basic modules (i.e., TDB, GES5, POLY3 and POST) and type the ordinary command-lines. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.

- The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-PLOY3-POST calculation.

Pause Options

After this information is displayed, you are prompted:

```
ENFORCE A PAUSE AFTER PLOTTING WHEN RUNNING A MACRO? /N/:
```

If you answer `Y` the following options are displayed.

```
1. START A COMPLETELY NEW POURBAIX DIAGRAM CALCULATION
2. OPEN AN OLD FILE & PLOT OTHER PROPERTY DIAGRAMS
3. OPEN AN OLD FILE & MAKE ANOTHER POURBAIX CALCULATION
4. OPEN AN OLD FILE & MAKE ANOTHER STEPPING CALCULATION
```

Option 1: Start a completely new POURBAIX diagram calculation

Make a completely new POURBAIX diagram calculation and automatically plot a pH-Eh diagram. i.e., define a new chemical system; specify the T-P-X conditions; calculate the initial equilibria; perform the pH-Eh mapping calculation; plot pH-Eh & various property diagrams.

```
CONSIDER THE GAS PHASE IN CALCULATING A POURBAIX DIAGRAM? /Y/

USE SINGLE DATABASE? /Y/:

COMBINED DATABASE: /PAQ2/:
```

DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION:

Normally a POURBAIX diagram and related equilibrium property in a heterogeneous interaction system are calculated under a certain bulk composition which is usually 1 kg of water with defined amounts of dissolving solute substances. The solutes may either be completely dissolved into the aqueous solution, or be partially dissolved and simultaneously form some solid phases.

CHEMICAL SYSTEM (ELEMENTS):

Default defined elements (solvent H2O): H & O and specially assigned ZE(electron) & VA(vacancy).

Prompt specified elements (solutes ELEM): Fe Ni Co Cr C N S Na Cl

INITIAL BULK COMPOSITION: Default defined composition (solvent): 1.0 kg of H2O

Prompt specified composition (solutes): x mole of ELEM

Notes: For accepting a default value, just RETURN at prompt;

For changing to a specific value, enter it at prompt.

IMPORTANT NOTE for Entering Solutes in Chemical Formulas:

First element letter in UPPER case, and second lower case! such as NaCl CO2 CoCl3 Fe0.93S NaSO4-1 H2SO4

Mass of Water (weight) = 1 kg

Option 2: Open an old file and plot other property diagrams

Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and just selectively plot other property diagrams. i.e., open the old GES and POLY3 workspaces; plot pH-Eh or various property diagrams.

```
FILE NAME /POURBAIX/

X-AXIS VARIABLE: /PH/:

Y-AXIS VARIABLE: /EH/:

CHANGE AXIS TYPE? /N/:

ZOOM IN? /N/:

CHANGE CURVE-LABEL OPTION FOR THE DIAGRAM? /N/:

ADD LABEL-TEXTS ONTO THE SPECIFIED DIAGRAM? /N/:
```

```
CHANGE THE SUBTITLE OF THE DIAGRAM? /N/:
CHANGE AXIS-TEXTS? /N/:
FURTHER REFINE THE DIAGRAM IN POST MODULE? /N/:
HARD COPY OF THE DIAGRAM? /N/:
SAVE X-Y COORDINATES OF CURVE ON TEXT FILE? /N/:
MODIFY THE DIAGRAM? /N/:
ANY MORE DIAGRAM? /N/:
```

Option 3: Open an old file and make another POURBAIX calculation

Open an existing POLY3 file created by POURBAIX Module and make another POURBAIX diagram calculation i.e., open the old GES and POLY3 workspaces; adopt the defined chemical system; modify the T-P-X conditions; calculate the initial equilibria; perform the pH-Eh mapping calculation; plot pH-Eh & various property diagrams.

```
CONSIDER THE GAS PHASE IN CALCULATING A POURBAIX DIAGRAM? /Y/:
FILE NAME /C:\USERS\AMANDA\DOCUME~1\POURBA~1.POL/:
ENFORCE GLOBAL MINIMIZATION TECHNIQUE IN CALCULATIONS? /N/:
SAVE ALL FUNCTIONS, VARIABLES AND TABLES IN POLY3 FILE? /Y/:
SET NUMERICAL LIMITS? /N/:
SET CALCULATING PARAMETERS:
LIST OF DEFAULT AND PRE-DEFINED CALCULATION CONDITIONS:
  UNITS: T IN K, P IN PASCAL, B(H2O) IN GRAM, N(ELEM) IN MOLE
T=298.15, P=1E5, B(H2O)=1000, N(H+1)=0, N(ZE)=0
DEGREES OF FREEDOM 0
CONFIRM DEFINED CONDITIONS? /Y/:
```

Additional Information About Option 3

The default definitions of the Eh and pH quantities in the advanced POURBAIX-Module (and in the ordinary TDB-GES-POLY calculation routines) should ALWAYS be as below:

```
Eh = MUR(ZE)/RNF
pH = -log10[AI(H+1,AQUEOUS)]
= -log10[ACR(H+1,AQUEOUS)*AH2O]
```

where RNF is the Faraday constant (96485.309 C/mol), and AH2O is the molecular weight of H2O (55.508435 g). MUR(ZE) is the electrochemical potential (ECP; in the unit of J/mol; w.r.t. the standard hydrogen electrode). ACR(H+1,AQUEOUS) is the site-fraction-based activity of the H+1 aqueous species in AQUEOUS solution phase, but AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH2O] is the molality-based activity of the H+1 aqueous species that should be used for defining the pH quantity.

Within an aqueous-bearing heterogeneous interaction system, the fundamental system-components must be H2O, H+1 and ZE, which are corresponding to the basic elements O & H and the hypothetical electron (ZE) in the aqueous solution phase. For the additional chemical elements in the system, their corresponding system-components shall be defined as in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S) or (for some) in their molecular forms (e.g., NaCl, H2S). The reference state for the H2O component must always be defined as the solvent species H2O in the AQUEOUS solution phase under the current temperature (*) and 100000 Pascal (i.e., 1 bar). The reference states for the H+1 and ZE components are by default set as their SER.

Various conventional properties of aqueous solute species I are converted in the following manners:

```
ML = Y(AQUEOUS,I)*AH2O/YH2O

RC = ACR(I,AQUEOUS)*YH2O/Y(AQUEOUS,I)

AI = RC*ML

= ACR(I,AQUEOUS)*AH2O
```

where YH2O [i.e., Y(AQUEOUS,H2O)] and Y(AQUEOUS,I) are the site-fractions of solvent H2O and solute species I.

LIST THE DEFINED AXIS-VARIABLES:

```
Axis No 1: LNACR(H+1)Min: -34.532525Max: 2.3025851 Inc: 0.8

Axis No 2: MUR(ZE)   Min: -150000   Max: 200000    Inc: 7718.85
```

NOTE: The default settings (listed above) for two mapping variables [in terms of lnACR(H+1) and MUR(ZE), and their minimum/maximum values and increment steps] are covering the following pH-Eh ranges/steps:

```
pH:  0.00 -> 14.00, at a step of 0.35

Eh: -1.55 ->  2.07, at a step of 0.08 (V)
```

The maximum pH limit has been calculated precisely and determined automatically by the POURBAIX-Module, as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system.

```
ACCEPT THE DEFAULT SETTINGS FOR TWO MAPPING VARIABLES? /Y/:

ANY MISSING PHASE BOUNDARY YOU COULD POSSIBLY THINK OF? /N/:

CHANGE THE PH/EH STEPS FOR SMOOTHER CURVES? /N/:

ZOOM IN? /N/:

CHANGE CURVE-LABEL OPTION FOR THE DIAGRAM? /N/:

ADD LABEL-TEXTS ONTO THE POURBAIX DIAGRAM? /N/:

CHANGE THE SUBTITLE OF THE DIAGRAM? /N/:

CHANGE AXIS-TEXTS? /N/:

FURTHER REFINE THE DIAGRAM IN POST MODULE? /N/:

HARD COPY OF THE DIAGRAM? /N/:

SAVE X-Y COORDINATES OF CURVE ON TEXT FILE? /N/:

MODIFY THE DIAGRAM? /N/:

ANY MORE DIAGRAM? /N/:
```

Option 4: Open an old file and make another STEPPING calculation

Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and make a normal STEPPING calculation. i.e., open the old GES and POLY3 workspaces; adopt the defined chemical system; specify one of the T-P-X conditions as the stepping variable; calculate the initial equilibria; perform the stepping calculation; plot various property diagrams.

Because of that in a STEPPING calculation will change some system definitions in a POURBAIX-type POLY3 file, it is highly advisable to make a backup of the existing POURBAIX-type POLY3 file (which you are going to open in this STEPPING calculation) before you proceed the further steps; otherwise, the structure of the loaded POLY3 file will be alternated by the option "4", and consequently the existing POLY3 file may be not suitable for other POURBAIX-type calculation any longer. Therefore, if you have not done so, you should make the copy right now!

However, a POLY3 file which is modified by this option can be further used for another STEPPING calculation inside the POURBAIX Module (by a repeated Option 4) or in normal POLY3 Module.

```
FILE NAME /C:\USERS\AMANDA\DOCUME~1\POURBA~1.POL/:

ENFORCE GLOBAL MINIMIZATION TECHNIQUE IN CALCULATIONS? /N/:

SAVE ALL FUNCTIONS, VARIABLES AND TABLES IN POLY3 FILE? /Y/:

SET NUMERICAL LIMITS? /N/:

   SET CALCULATING PARAMETERS:

   List of Default and Pre-defined Calculation Conditions:

   --------------------------------------------------------------

     Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole

   --------------------------------------------------------------

   T=298.15, P=1E5, B(H2O)=1000, N(H+1)=0, N(ZE)=0

   DEGREES OF FREEDOM 0

FURTHER MODIFY SYSTEM DEFINITIONS & CONDITIONS IN POLY3 MODULE? /N/:

CONFIRM DEFINED CONDITIONS AS THE STARTING POINT? /Y/:
```

The following parameters are suitable for a STEPPING calculation for the defined aqueous-bearing system. Choose one of them as the stepping variable:

```
   T Temperature (C)

   P Pressure (bar)

   pH Acidity

   Eh Electronic Potential (V)

   N(Comp) Mole of One Component
```

where "Comp" is the name of a specific component as listed below. One should not use any key component (H2O or H+1 or ZE) as such a stepping variable, because of that their compositional definitions and variations are determined by the AQUEOUS solution phase in the POURBAIX Module.

An interacting component defined as an element (such as Fe or Na or Cl) can be selected as a stepping variable.

However, if you want to make a stepping calculation with a non-element chemical formula (such as NaCl or CaS2) as the stepping variable, one must have made some necessary modifications in the POLY3 Module, before reaching this point, by conducting some POLY3 commands as given below (as an example for the system Fe-Na-Cl-H-O):

```
POLY_3: def-component H2O H+1 ZE Fe NaCl Cl
POLY_3: set-ref-state H2O AQUEOUS * 1E5
POLY_3: set-ref-state ZE REF_ELEC * 1E5
POLY_3: change-status phase REF-ELEC=SUSPEND
POLY_3: set-cond b(H2O)=1000 n(H+1)=0 n(ZE)=0
POLY_3: set-cond P=1E5 T=298.15**
POLY_3: set-cond n(Fe)=1E-3 n(Cl)=0 n(NaCl)=3 **
```

** Here the P-T-n(Fe) conditions can be set as what you wanted, while the initial n(NaCl) value must be set as between its minimum and maximum values that you are interested in. Later on, it will be prompted for specifying the n(NaCl) Min-Max-Step values of the stepping calculation.

```
STEPPING VARIABLE: /T/:
MINIMUM TEMPERATURE (C) /15/:
MAXIMUM TEMPERATURE (C) /35/:
INCREMENT IN TEMPERATURE (C) /1/:
CHANGE AXIS TYPE? /N/:
ZOOM IN? /N/:
CHANGE CURVE-LABEL OPTION FOR THE DIAGRAM? /N/:
ADD LABEL-TEXTS ONTO THE SPECIFIED DIAGRAM? /N/:
CHANGE THE SUBTITLE OF THE DIAGRAM? /N/:
CHANGE AXIS-TEXTS? /N/:
FURTHER REFINE THE DIAGRAM IN POST MODULE? /N/:
HARD COPY OF THE DIAGRAM? /N/:
SAVE X-Y COORDINATES OF CURVE ON TEXT FILE? /N/:
MODIFY THE DIAGRAM? /N/:
ANY MORE DIAGRAM? /N/:
```

REACTOR_SIMULATOR_3 Commands

In this section:

CREATE_DIVIDERS

Define the segment boundaries and the ways on how to distribute phases between various segments and to split the feeds of heat and mass.

Syntax	CREATE_DIVIDERS
Prompts	`NUMBER OF DIVIDERS /4/: <THE NUMBER OF DIVIDERS>` Specify the number of dividers (boundaries between various segments) in the reactor. It is normally the segment number plus one: for example, if the stage box number is defined as 4, the divider number should be defined as 5.
	`NUMBER OF OUTPUTS FOR DIVIDER # /3/: <THE NUMBER OF OUTPUTS>` Specify the number of outputs for a specific divider #.
	`PERCENT OF INPUT TO OUTPUT 1 /100/: <PERCENT OF INPUT>` Define the percentage of input to the output 1 in the current divider #.
	`PERCENT OF INPUT TO OUTPUT ## /100/: <PERCENT(S) OF INPUT(S)>` Define the percentages of inputs to the outputs ## in the current divider #. It is repeated till the last output is specified.

CREATE_PIPES

Define the pipes between various segments and the ways on how the mass and heat transport between the surroundings (with the record number as 0) and the reactor, among various segments in the reactor, and along various dividers (segment boundaries in the reactor).

Syntax	CREATE_PIPES
Prompts	`FROM RECORD: <A RECORD NUMBER>` Specify a record number. If there are four segments in the reactor, these records are available: • `0` surroundings • `1-4` stage boxes (segments) • `5-9` dividers (segment boundaries)
	`PIPE TO RECORD: <ANOTHER RECORD NUMBER>` Specify another record number to which the mass or heat flows from the current record (specified above). Before this prompt, a message shown on the screen indicates what kind of mass or heat flow (according to the definitions of stage boxes and dividers, which have already been created prior to this command) should be specified in the pipe. This is

Syntax	CREATE_PIPES
	repeated for all inputs and/or outputs for mass and/or heat in current record.

CREATE_STAGE_BOXES

Create several reaction stages as boxes (segments), where the you define the feed in either mass input and initial temperature or heat input from surroundings, as well as the mass out and initial temperature in each of the segments.

Syntax	CREATE_STAGE_BOXES
Prompts	`NUMBER OF STAGE BOXES /4/: <THE NUMBER OF STAGE BOXES>` Specify the number of stage boxes in the reactor. Then define the feed of mass and/or energy (from surroundings to) the rector.
	`GIVE FEED TO SYSTEM: <FEED>` One feed (of mass or heat) to the reactor must be specified here. Two types of feeds can be used: • As input amount of heat (enthalpy): `H=Value`. • As input amount of specific species or element and its initial temperature: `N(SPECIES)=Value, Input temperature` (in one line, or the input temperature in the next prompt).
	`INPUT TEMPERATURE /298.15/: <INPUT TEMPERATURE>`

	`GIVE FEED TO SYSTEM: <FEED>`
	Specify other feeds (mass or energy) to the reactor. Press <Enter> to finish the feed inputs, and then:
	`GIVE FOR STAGE BOX #`
	Now start to define the type of stage box (segment is specifically numbered as #), and to specify a guess of initial temperature and an output for each phase in the segment.

	`TYPE OF BOX /EQUILIBRIUM/: <TYPE OF BOX>` Only the `EQUILIBRIUM` type is allowed. Press <Enter> to accept it.
	`IS THE STAGE HEAT CONTROLLED? /Y/: <YES OR NO>` `Y` means the current segment is heat controlled.
	`INITIAL GUESS OF TEMPERATURE? /1000/: <INITIAL TEMPERATURE>` Give a guess of initial temperature (in K) for the current segment; press <Enter> to accept

Syntax	CREATE_STAGE_BOXES
	the default.
	`GIVE INITIAL AMOUNT: <INITIAL AMOUNT OF MASS OR HEAT>` The initial amount of mass and/or heat in the current segment can be specified here. Two types of initial amount can be used: • As initial amount of heat (enthalpy): `H=Value`. • As initial amount of specific species or element and its initial temperature: `N(SPECIES)=Value, Input temperature` (in one line, or the input temperature in the next prompt).
	`INPUT TEMPERATURE /298.15/: <INPUT TEMPERATURE>`

	`GIVE INITIAL AMOUNT: <INITIAL AMOUNT OF MASS OR HEAT>`
	Specify initial amount (mass or energy) in the current segment. Press <Enter> to finish the initial amount inputs, and then this message displays:
	`Each phase may have a separate output, give these`
	Now start to define the output for each phase.

	`PHASE NAME /REST/: <NAME OF PHASE>` Specify a phase that has a separate output, e.g. `GAS`; by pressing <Enter> to accept that all `REST` phases do not have separate outputs. Then the program asks for further definitions of all the other segments (one by one), repeating some of the above questions, till the last segment in the reactor is defined.

EXECUTE_POLY3_COMMAND

Syntax	EXECUTE_POLY3_COMMAND
	To directly use all kinds of POLY commands inside the REACTOR module. Any legal *POLY_3 Commands* on page 117 can be entered.

LIST_RECORDS

Syntax	LIST_RECORDS
	Lists all the already-created records for the reactor (including stage boxes, dividers, pipes, etc.).

READ_WORKSPACE

The REACTOR workspace (along with the related POLY3 and GIBBS workspaces) and the simulated results from the SIMULATE command can be read by this command from a binary file where they must be saved with *SAVE_WORKSPACE* below. The *.RCT file is not printable.

Syntax	READ_WORKSPACE
Options	`File name`: The name of a saved *.RCT file where the REACTOR and POLY3/GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default .RCT, otherwise type the whole *.RCT file name. An **Open** window displays if a file name is not given after the command or its path is incorrect, so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** (i.e. RCT) cannot be changed.

SAVE_WORKSPACE

The REACTOR (and POLY3/GIBBS) workspaces are saved on a file with this command. In the GIBBS workspace, all thermochemical data are stored. In the POLY3 workspace, all thermochemical data, all conditions, changed status, entered symbols, etc., are stored. In the REACTOR workspace, all definitions of multi-stage steady-state rector and its distribution coefficients are saved, together with the GIBBS and POLY3 workspaces. After a SAVE command, you can always return to the state when you issued the SAVE command by giving a READ command.

After saving the REACTOR (and POLY3/GIBBS) workspaces on a file, you can leave the program and at a later time READ the file and continue from the saved state.

A START_SIMULATE command automatically saves on the work file with the most lately specified name. To avoid destroying the simulated results, do not SAVE after a START_SIMULATE command is enforced, similar to that you should not SAVE after a STEP or MAP command! You may append several results by START_SIMULATE without destroying the previous results but SAVE erases them all.

Syntax	SAVE_WORKSPACE
	`FILE NAME` A file name must be specified. The default extension of the RCT file is .RCT, while or any other extension as required.
	A **Save** window displays if a file name is not given after the command, so that the path (in the **Save in** field) and **File name** can be specified. The **Files of type** (i.e. RCT) cannot be changed. If there is already a file with the same file name under the directory a warming message displays. Click **OK** to overwrite the current REACTOR (and POLY3/GIBBS) workspaces onto the existing *.RCT file. Click **Cancel** to return to the REACTOR module. You

Syntax	SAVE_WORKSPACE
	can use the SAVE command with an unspecified name (i.e. through `SAVE ,,,` command-sequence) to save the REACTOR (and POLY3/GIBBS) workspaces.

START_SIMULATION

Start the reactor simulation, and list the results for all iterations. The output for each iteration consists of the conditions set in each segment, and you can also select some state variables to list. After each loop, the temperatures in all segments are listed.

Syntax	START_SIMULATION
Prompts	`MAX NUMBER OF LOOPS /10/: <THE MAX NUMBER OF LOOPS>` Give the max number of loops. The REACTOR module repeats the reactor simulation until this loop number is reached.
	`OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME OR RETURN>` Decide on either listing simulation results on the screen (by pressing <Enter>) or saving them on an experimental file (with the default extension .EXP). The conditions in each segment are not saved in the file, only on the screen.
	`OUTPUT VARIABLES /T BP($)/: <VARIABLE NAME(S)>` Specify the variable name(s) that is also listed on the screen together with the conditions in each segment, or in the output experimental file.

Example Output

For a four-stage reactor, the output at a certain iteration may look like this:

```
H=-991745.1, P=100000, N(C)=2.8468936, N(N)=6.78399966E-4, N(O)=3.8171615,

N(SI)=1.77031

DEGREE OF FREEDOM 0

BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588099,

BP(QUARTZ_S3)=68.193896

1.78803E+03

BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03

BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292

2.08691E+03

BP(GAS)=71.23129, BP(SI_L)=22.471787

2.20831E+03
```

```
H=-924751,87, P=100000, N(C)=2.0594558, N(N)=5.17999978E-4, N(O)=4.0142358,
N(SI)=2.7551438
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588098,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=-813239., P=100000, N(C)=1.6592668, N(N)=3.59999988E-4, N(O)=3.7549293,
N(SI)=2.896635
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588098,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=7374.6403, P=100000, N(C)=8.84911857E-1, N(N)=1.99999996E-4, N(O)=1.9379203,N
(SI)=1.853872
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175982, BP(C_S)=8.1588097,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
10  1788.03  2065.69  2086.91  2208.31     0.00     0.00     0.00
```

SCHEIL Commands

Search the online help or see the *Thermo-Calc User Guide* included with this PDF documentation set for details about how to calculate using Scheil either in Graphical Mode (the Scheil Calculator) and Console Mode (the wizard Scheil module).

If you also have a license for the Diffusion Module (DICTRA), you can import a previously calculated Scheil segregation profile into the software using the command INPUT_SCHEIL_PROFILE. Search the online help or see the *Diffusion Module (DICTRA) Command Reference Guide*.

In this section:

BCC_TO_FCC_TRANSFORMATION

Use this command for the Scheil module to allow transformations in the solidified part of the alloy caused by each of the components specified to be Fast Diffuser. It is recommended that you only select this for steels.

Syntax	BCC_TO_FCC_TRANSFORMATION
Prompt	`ALLOW BCC 🕚 FCC ? /N/` The default is `N`. Enter `Y` to allow transformations.

EVALUATE_SEGREGATION_PROFILE

Use this command in order to evaluate a segregation profile while performing the Scheil calculation. The Scheil calculation itself does not contain a spatial dimension. However, if it is assumed that the molar volume is constant and equal for all elements, and if a length is provided over which solidification occurs (for example the secondary dendrite arm spacing) then the generated profile corresponds to the segregation that would be obtained under the assumptions of a Scheil calculation. The grid is then equidistant and can be used as input for a DICTRAsimulation.

The generated text file contains, on each line, the mole fractions of all elements in alphabetical order at a certain grid point. If the composition is the same on several consecutive lines it means that the composition of the then remaining liquid has reached a state in which there are no degrees of freedom.

Syntax	EVALUATE_SEGRATION_PROFILE
Prompt	`EVALUATE SEGREGATION PROFILE? /N/` If the answer is `Y`a segregation profile will be evaluated and saved to disc. Note that this feature is not supported with back diffusion; if back diffusion is enabled no segregation profile will be generated.
	`NUMBER OF GRID POINTS /100/` Enter the number of grid points for the segregation profile. A file dialogue window opens and allows you to specify the name of the file in which the segregation profile is written. In a macro file it is possible to enter all arguments on a single line, e.g. `EVALUATE_ SEGREGATION_PROFILE Y 100 XF.TXT`, meaning that the segregation profile is evaluated over 100 grid points and saved to a file (XF.TXT) in the current working directory.

GLOBAL_MINIMIZATION

Use this command for the Scheil module to use global minimization.

Also see the POLY commands topic *ADVANCED_OPTIONS Descriptions* on page 120 for information about that GLOBAL_MINIMIZATION command.

Syntax	GLOBAL_MINIMIZATION
Prompt	`USE GLOBAL MINIMIZATION? /N/` If `Y`, the Global Minimization is done when possible (depending on the conditions setting), and a Global Minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust. If `N` the Global Minimization is not used to reach the equilibrium.

LIQUID_PHASE_NAME

Use this command for the Scheil module to use the liquid phase name from the database definitions or enter another phase name.

Syntax	LIQUID_PHASE_NAME
Prompt	`LIQUID PHASE NAME /DEFAULT/` Default selects the liquid phase from the database definitions, otherwise enter a phase name.

SAVE_FILE_NAME

Use this command for the Scheil module to save the file. The files get the console number added to this name, e.g. 005.->Scheil_006.poly3 and Scheil_segregation_profile.txt).

Syntax	SAVE_FILE_NAME
Prompt	Name of files to be saved, poly3 and segregation profiles.

SET_INTERACTIVE

Syntax	SET_INTERACTIVE
	Resets the input and output units to the initial values, i.e. keyboard and screen. Add this as the last command to the macro files.

SET_NUMERICAL_LIMITS

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by *COMPUTE_EQUILIBRIUM* on page 139, *STEP_WITH_OPTIONS* on page 172, *MAP* on page 158 or *ADVANCED_OPTIONS* on page 125), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30 to hardware
precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current Thermo-Calc (Console Mode) run, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	`MAXIMUM NUMBER OF ITERATIONS /200/: <XXX>` By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
	`REQUIRED ACCURACY /1E-6/: <YYY>` This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
	`SMALLEST FRACTION /1E-12/: <ZZZ>` This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is `1E-12` for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as `1E-30` (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system).
	`APPROXIMATE DRIVING FORCE CALCULATION FOR METASTABLE PHASES /Y/: <Y OR N>` Normally the POLY module only requires that the set of stable phases is in equilibrium in order to terminate the iterations. The metastable phases are included in all iterations but these may not have reached their most favourable composition and thus their driving forces may be only approximate [corresponding to `Y`]. You can also force the calculation to converge for the metastable phases by answering `N` if it is important that these driving forces are correct, which may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.

START_WIZARD

Use this command for the Scheil module to use the wizard with step-by-step prompts to create a Scheil simulation.

This wizard walks you through a basic Scheil simulation. You are prompted for settings including the major element or alloy, composition input in mass (weight) percent, the alloying elements, the temperature, fast diffusing components, and whether any phase should have a miscibility gap check.

Use the other commands to make changes to settings that are not included in this wizard.

- BCC_TO_FCC_TRANSFORMATION
- EVALUATE_SEGREGATION_PROFILE
- GLOBAL_MINIMIZATION
- LIQUID_PHASE_NAME
- SAVE_FILE_NAME
- STORED_COMPOSITION_TYPE
- TEMPERATURE_STEP
- TERMINATION_CRITERIA

Syntax	START_WIZARD

Prompt	`DATABASE /<DEFAULT>/:`
	`MAJOR ELEMENT OR ALLOY:`
	`COMPOSITION INPUT IN MASS (WEIGHT) PERCENT? /Y/:`
	`1ST ALLOYING ELEMENT:CR 10 C 1`
	`NEXT ALLOYING ELEMENT:`
	`TEMPERATURE (C) /2000/:`
	`FAST DIFFUSING COMPONENTS: /NONE/:C`
	`SHOULD ANY PHASE HAVE A MISCIBILITY GAP CHECK? /N/:`

TEMPERATURE_STEP

Use this command for the Scheil module to define a temperature step.

Syntax	TEMPERATURE_STEP
Prompt	`SET TEMPERATURE STEP (C) /1/`

TERMINATION_CRITERIA

Use this command for the Scheil module to define the termination criteria for the fraction of liquid or temperature.

Syntax	TERMINATION_CRITERIA
Prompts	`FRACTION OF LIQUID OR TEMPERATURE (F OR T)? /F/`
	`FRACTION OF LIQUID /.01/`

SYSTEM_UTILITIES Commands

In this section:

ABOUT

Syntax	ABOUT
	Lists basic information about the development history and ownership of the Thermo-Calc software and its components.

CLOSE_FILE

Close an opened text file.

Syntax	CLOSE_FILE
Prompt	`UNIT NUMBER: <UNIT NUMBER>` A unit number given in an OPEN_FILE command must be specified.

DISPLAY_LICENSE_INFO

Use this command to launch a license diagnostics program implemented in the SYS module. It detects the license information for the Thermo-Calc installations on the current client computer (and on the connected license server), and lists the details, including the current status of available license file and all its included license features for the current installation(s), as well as the Safenet Environment Variables and detailed Local (Client) Information, on screen or into a textual file (*.TXT).

This is useful for a list of license details, and to obtain basic technical support by sending the *.TXT file to support@thermocalc.se. If you are running a network client installation of Thermo-Calc, you can see how many of the client example licenses that are currently checked out and how many of them are left. You can also see which clients computers it is that have checked these client example licenses out.

Syntax	DISPLAY_LICENSE_INFO
Prompt	`OUTPUT TO SCREEN OR FILE /SCREEN/: <MYLICENSEINFO.TXT>` Press <Enter> to display a list of license information or into a *.TXT file under a specific file name which can later on be opened and edited by any basic text editor.

HP_CALCULATOR

This is the QBA simple interactive calculator using reverse Polish notations.

Syntax	HP_CALCULATOR
	Available OPCODEs (HPC codes) are listed by entering the command HELP. Use the BACK command to quit the HP_CALCULATOR and go back to the SYS module. Input are numbers, + - * / and ^ and OPCODEs. Several numbers an operations can be given on one line. The content of the X register is displayed after each operation. For example, to compute 2*EXP(1.5**3-30000/(8*1273)), you should input the following: `30000 8/1273/chs 1.5 3 ^ + exp 2 *`

OPEN_FILE

A text file is opened for use in other commands where a unit number is necessary. The program automatically assigns a unit number.

Syntax	OPEN_FILE
Prompt	`FILE NAME: <FILE NAME>` A legal file name must be specified.

SET_COMMAND_UNITS

This command is useful for reading inputs already prepared by a textual editor on a file. Such inputs can be a table of values or a large number of parameters. The file must be opened with *OPEN_FILE* above.

The first two lines of an input file are skipped before any input is read.

Syntax	SET_COMMAND_UNIT
Prompt	`INPUT UNIT NUMBER /5/: <INPUT UNIT NUMBER>` Specify the input unit number returned from an OPEN_FILE command. The next command is taken from the file connected to this unit number. The last command on such a file must be EXIT or SET_INTERACTIVE when you are in POLY, POST or SYS module, in order to go back to read input from the keyboard. The default value is the current input unit.
	`OUTPUT UNIT NUMBER /6/: <OUTPUT UNIT NAME>` Specify the output unit number returned from an OPEN_FILE command.

SET_ECHO

Syntax	SET_ECHO
	Add this command at the beginning of a Console Mode MACRO *.TCM file (or to the primary MACRO file on the top level if any sub-level(s) of MACRO files are used). Automatically displays on screen the complete details of various commands in all the sequential operations in the software, that are enforced according to the MACRO file(s). This command is not applicable if MACRO files are not used.

SET_INTERACTIVE_MODE

Syntax	SET_INTERACTIVE_MODE
	Resets the input and output units to their initial values, i.e. keyboard and screen. Remember to add this as the last command to your MACRO files, in order to stop execution of the command file in the POST module. It has no meaning in interactive mode.

SET_LOG_FILE

Use it to save, in a basic text file, everything typed in the Thermo-Calc software. When having problems executing a command sequence, this command can be used to save the command typed onto a log file. The manager can then check what the problem might be.

This command also makes the system echo the full command for all commands typed. This feature is useful when demonstrating the system since the abbreviated commands are often difficult.

The saved log file can then be edited as a MACRO file by using a basic text editor. This is useful to run the MACRO file(s) for similar calculations (the same system but slightly varied temperature-pressure-composition conditions), or run the example MACRO files.

Syntax	SET_LOG_FILE
Prompt	A **Save** window opens to specify a file name for the *.LOG file, so that the path (in the **Save in** field) and **File name** can be specified. If an *.LOG file with the same name exists in the current working directory, it is overwritten. The **Files of type** (i.e. LOG) cannot be changed. Click **Save** or **Cancel** as applicable.

SET_PLOT_ENVIRONMENT

Allows you, preferably in the initiation file tc.ini, to set the plot devices you normally have access to as this can vary for different Thermo-Calc installations.

> This command must be terminated with an empty line or two commas.

Syntax	SET_PLOT_ENVIRONMENT
Prompts	`DEFAULT PLOTDEVICE NUMBER /DEFAULT NUMBER/: <DEVICE NUMBER>` The number given is unique for each type of graphical device. For plotting various types of Thermo-Calc graphs on screen, the default graphical device number should normally be selected. A question mark ? gives you a list of all available graphical devices used in the Thermo-Calc Console Mode.
	`PSEUDO FILE NAME: <PSEUDO-FILE NAME>` The name given here is a symbol which can be used to refer to a physical graphics device when asked for graphical output file.
	`PLOTDEVICE NUMBER /1/: <DEVICE NUMBER>` The number that specifies the type of graphical device.

	`PLOT FILE NAME: <FILE NAME OR PRINTER NAME>`
	The name of the graphical device on system level (name of file or printer).
	Example
	`SET_PLOT_ENVIRONMENT 1 lasp 5 a0tr,,`
	This example sets the default plot device number to `1`, and defines an alias named `lasp` with plot device `5` and connected to a printer named `a0tr`.

SET_TC_OPTIONS

Predefine the default values of three general Thermo-Calc options for performing all the sequential single-points, stepping and mapping calculations.

Syntax	SET_TC_OPTIONS
Prompts	`USE_GLOBAL_MINIMIZATION /YES/: <Y OR N>` If `Y`, it is done when possible (depending on the conditions setting), and a Global Minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust. For `N` Global Minimization is not used to reach the equilibrium.
	`GLOBAL_TEST_INTERVAL /0/: <AN INTEGER VALUE>` The integer number determines how often the Global Minimization should be used during calculations with *STEP_WITH_OPTIONS* on page 172 and *MAP* on page 158. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during STEP calculations, and only at node points during MAP calculations. Any other positive integer number, n, suggests it performs Global Minimization tests at every nth step during STEP and MAP calculations. Of course, the Global Minimization test is always carried out at a phase change or a node point. The Thermo-Calc Console Mode is initially configured with 0 (zero) as the default value, but such a configuration for the default value can be changed by this option.
	`AUTOMATICALLY_ADD_INITIAL_EQUILIBRIA /YES/: <Y OR N>` When *ADD_INITIAL_EQUILIBRIUM* on page 119 is not used before a MAP calculation, a mesh of INITIAL_EQUILIBRIUM are automatically added before the mapping procedure itself takes place. This mesh is only available when the two independent axis-variables have already been defined by the POLY command.
	`SET_AXIS_VARIABLE` For `Y` the POLY module always enforces the automatic procedures for adding initial equilibrium points during mapping. For `N` no initial equilibrium points are then added during mapping.

STOP_ON_ERROR

Useful for batch jobs in order to prevent that an erroneous sequence of commands to the program causes waste of computer activity.

Syntax	STOP_ON_ERROR
	Give the preferred argument (`ON` or `OFF`) after the STOP command. If the default argument ON is given, the program terminates after an illegal or ambiguous command. It is possible to reset the effect of this command by giving the argument OFF.

TABULATION_REACTION Commands

In this section:

ENTER_FUNCTION

Used to define a new thermodynamic function to be included in the sixth column of tabular output. The last entered function is listed in the 6th column of all tables, and can be plotted (if choosing the Plot Column value 6) in all graphs, for all subsequently tabulated substances or reactions.

Syntax	ENTER_FUNCTION
Prompt	`NAME: <NAME>` `FUNCTION: <DEFINITION>`
	A limited number of state variables, G, H, S, T, P, V and H298 can be used in the function definition. For example, -(G-H)/T can be defined as a function which is identical to S for a substance or ΔS for a reaction, G+T*S-P*V can be defined as a function which is U (internal energy) for a substance or ΔU (internal energy change) for a reaction.
Options	`Name`of the function (maximum 8 characters) and `Definition` of the function. A long function can be typed over several lines. A function should be terminated by a semicolon (;) or an empty line.

Example Output

For the pure substance Fe (using the SSUB database), by entering a function as `G+T*S-P*V`, the following table is obtained by typing <Enter> in the prompt `Output file /SCREEN/:`, and the figure by typing `6` in the prompt `Plot column /2/:`

```
TAB: ENTER-FUNCTION

Name: InEnergy

Function: G+T*S-P*V;

TAB: TABULATE_SUBSTANCE

Substance (phase): Fe

Pressure /100000/: <Enter>

Low temperature limit /298.15/: <Enter>

High temperature limit /2000/: <Enter>

Step in temperature /100/: <Enter>

Output file /try1/: try2

Graphical output? /Y/: <Enter>

Plot column? /2/: 6
```

This gives the following output:

```
O U T P U T   F R O M   T H E R M O - C A L C

Column 6: InEnergy G+T*S-P*V

Phase : FE_S                       Pressure :      100000.00
```

```
Specie: FE
**************************************************************
    T      Cp             H             S             G             InEnergy
   (K)    (Joule/K)      (Joule)       (Joule/K)      (Joule)
**************************************************************
  298.15   2.48446E+01   2.17972E-06   2.72800E+01  -8.13353E+03   2.17972E-06
  300.00   2.48905E+01   4.60049E+01   2.74338E+01  -8.18414E+03   4.60049E+01
  400.00   2.71299E+01   2.64957E+03   3.49085E+01  -1.13138E+04   2.64957E+03
  500.00   2.93561E+01   5.47211E+03   4.11976E+01  -1.51267E+04   5.47211E+03
  600.00   3.19293E+01   8.53245E+03   4.67701E+01  -1.95296E+04   8.53245E+03
  700.00   3.50985E+01   1.18777E+04   5.19207E+01  -2.44667E+04   1.18777E+04
  800.00   3.92042E+01   1.55830E+04   5.68623E+01  -2.99068E+04   1.55830E+04
  900.00   4.49645E+01   1.97726E+04   6.17903E+01  -3.58387E+04   1.97726E+04
1000.00   5.42147E+01   2.46891E+04   6.69619E+01  -4.22728E+04   2.46891E+04
1100.00   4.55851E+01   2.99025E+04   7.19412E+01  -4.92328E+04   2.99025E+04 $ Stable
phase is FE_S2
1200.00   3.40840E+01   3.51037E+04   7.64466E+01  -5.66322E+04   3.51037E+04
1300.00   3.49398E+01   3.85549E+04   7.92086E+01  -6.44162E+04   3.85549E+04  1400.00
3.57994E+01   4.20918E+04   8.18293E+01  -7.24692E+04   4.20918E+04
1500.00   3.66636E+01   4.57149E+04   8.43287E+01  -8.07780E+04   4.57149E+04
1600.00   3.75330E+01   4.94247E+04   8.67226E+01  -8.93314E+04   4.94247E+04 $ Stable
phase is FE_S3
1700.00   4.05217E+01   5.41173E+04   8.95609E+01  -9.81363E+04   5.41173E+04
1800.00   4.12595E+01   5.82055E+04   9.18975E+01  -1.07210E+05   5.82055E+04 $ Stable
phase is FE_L
1900.00   4.60000E+01   7.74165E+04   1.02377E+02  -1.17099E+05   7.74165E+04  2000.00
4.60000E+01   8.20165E+04   1.04736E+02  -1.27456E+05   8.20165E+04
```

ENTER_REACTION

This is the same as *TABULATE_REACTION* on page 260 in that both the chemical reaction can be specified and the thermodynamic property changes for the reaction can be generated as a table, and plotted as a graph or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB5 database (by default), or the current database set by *SWITCH_DATABASE* on page 20 (thus there is no need to use the DATA module before this command). You can select any other database by using the SWITCH_DATABASE command in the TAB module. The rules to specify a reaction are the same as in the command TABULATE_REACTION.

Syntax	ENTER_REACTION
Prompts	`SAME REACTION? /Y/: <Y OR N>` This displays if there is at least one reaction already defined either by the command ENTER_REACTION or TABULATE_REACTION. For `Y` the next prompt for defining reaction is not asked.

	`REACTION: <CHEMICAL REACTION EQUATION> & <RA+RB=PC+PD>`
	A long reaction can be typed over several lines. A reaction should be terminated by a semicolon (;) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.:
	`Pressure /100000/: <pressure of interest, in pa>`
	`Low temperature limit /298.15/: <T-low, in K>`
	`High temperature limit /2000/: <T-high, in K> Step in temperature /100/: <T-step>`

	`OUTPUT FILE /SCREEN/: <RETURN FOR SCREEN, OR TYPE A FILE NAME>` If you type `Return for screen` a list of thermodynamic property changes for the defined/chosen reaction is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated. If typing a file name, the table is displayed and saved as an *.EXP or an *.TAB file. Then prompts:
	`GRAPHICAL OUTPUT /Y/: <Y OR N>` For `N` a table is output to the screen and this table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. For `Y` a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it further asks which column is to be plotted on the resulting graph:
	`PLOT COLUMN? /2/: <1 OR 2 OR 3 OR 4 OR 5 OR 6>` Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a `POST` prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the

Syntax	ENTER_REACTION
	X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the `POST` prompt always takes you back to the TAB module.

LIST_SUBSTANCES

List all species in the current database with a certain set of elements. This is useful to specify species as pure substances in the command *TABULATE_SUBSTANCE* on page 262.

Syntax	LIST_SUBSTANCES
Prompts	`WITH ELEMENTS /*/ <* OR A SET OF ELEMENTS>` The elements building up various species must be specified. The wildcard * means all elements in the current database. If some elements are specified, it also prompts for how to list species with such elements.
	`EXCLUSIVELY WITH THOSE ELEMENTS /Y/: <Y OR N>` All species (not phases) in the current database are searched. If the answer is `Y` (the default), no other elements are allowed in searching, except for those specified. If `N` all species containing at least one of the specified elements are listed.

Example Output

For the SSOL5 database, there are different lists, as shown below:

```
TAB: l-sub
With elements /*/: <Enter>
VA                      AG                      AL
AM                      AS                      AU
B                       BA                     BE BI  BR C
CA                      CD                      CE
CL                      CO                      CR
CS                      CU                      DY
ER                      EU                      F
FE                      GA                      GD
GE                      H                       HF
HG                      HO                      I
IN                      IR                      K
LA                      LI                      LU
MG                      MN                      MO
```

```
NA                      NB
ND                      NI                      NP
OS                      P
PA                      PB                      PD
PR                      PT                      PU
RB                      RE                      RH
RU                      S                       SB
SC                      SE                      SI
SM                      SN                      SR
TA                      TB                      TC
TE                      TH                      TI
TL                      TM                      U
V                       W                       Y
YB                      ZN                      ZR
C1                      C2                      C3
C4                      C5                      C6
C7                      N2                      O2
P1                      P2                      P4
NA/+1                   K/+1                    CL/-1
H2O                     H1/+                    LI1/+
CS1/+                   RB1/+                   O1H1/-
F1/-                    BR1/-                   I1/-
H1/+1                   H1O1/-1                 SI1O2 CA1O1 TAB:
TAB: l-sub
With elements /*/: fe cr ni c n o
Exclusively with those elements? /Y/: <Enter>
C               CR                    FE
N               NI                    O
C               C2                    C3
C          C5                    C6
C               N2                    O2
TAB:l-sub fe cr ni c n o
Exclusively with those elements? /Y/: n
C               CR                    FE N   NI O
C1              C2                    C3
C4              C5                    C6
```

```
C7            N2                 O2
H2O           O1H1/-             H1O1/-1 SI1O2 CA1O1 TAB:
```

SET_ENERGY_UNIT

Set the energy unit as calories or Joule, in all the subsequent outputs (tables, graphs, and files) in the current calculation operation.

Syntax	SET_ENERGY_UNIT
Prompt	`ENERGY UNIT (C=CAL, J=JOULE) /J/: <UNIT>`

SET_PLOT_FORMAT

Set the plotting format while the result is plotted on screen or the file is saved as EXP file [using DATAPLOT graphical format] and TAB file (as a basic text file and as displayed on screen).

This command is different from *SET_PLOT_FORMAT* on page 210 in the POST module, but is identical to *SET_PLOT_ENVIRONMENT* on page 245 in the SYS (system utility) monitor.

Syntax	SET_PLOT_FORMAT
Options	The default set `Unit` is `1` (Windows) or `9` (Linux) for graphical presentation on screen, or all other units for outputs as *.EXP and *.TAB files. Also set the format of the graphical output to different graphical devices. The default unit 22 (1 for legacy Windows, and 9 for legacy Linux) may be altered with the SET_PLOT_ENVIRONMENT command in the SYS monitor or by the TC.INI file.

SWITCH_DATABASE

By default, the TAB module always automatically retrieves thermodynamic data for substances or reactant/product substances in a defined reaction, or for pure phases or ideal solution phases, from the SSUB Substances Database. However, you can select thermodynamic data for complex non-ideal solution phases from another database. This is possible with this command.

This command switches (or changes) from the current database to a new one, and reinitializes the entire TAB module for defining a substance or reaction and the GIBBS workspace for storing retrieved data. All the directly connected databases as predefined by the original database initiation file (TC_INITD.TDB file in the /DATA/ area for Windows environments, or the initd.tdb file in the \data\ area for Linux) are listed by pressing the <Enter> key without giving any argument. You can also supply your own database by giving the argument USER and then the database name and, if it is not located in the current working directory, its correct path.

This command (when required to use another database for subsequent tabulations) must be used before executing the TAB commands *TABULATE_SUBSTANCE* on page 262 for substances, and *ENTER_REACTION* on page 249 or *TABULATE_REACTION* on page 260 for reactions.

When a predefined database or an appropriate USER database is switched on, the DATA command *GET_DATA* on page 15 is automatically executed; therefore, the TAB module immediately displays a message

Example

Example of TAB module message with the PSUB database specified

```
TAB: SW PSUB

THERMODYNAMIC DATABASE Module running on PC/Windows NT

Current database: TC Public Substances Database

VA DEFINED

REINITIATING GES5

VA DEFINED

ELEMENTS

SPECIES

PHASES

PARAMETERS

FUNCTIONS

-OK- TAB:
```

Syntax	SWITCH_DATABASE

Prompt	`DATABASE /XYZ/: <NEW DATABASE NAME>`
	Specify a `New database name`. `XYZ` stands for the default SSUB database or the current database which is switched on. If an appropriate database name is not given and the `USER` option is not used, this list displays:
	`Use one of these databases`
	`PURE4 = SGTE Pure Elements Database v4`
	`SSUB3 = SGTE Substances Database v3`
	`USER = user defined database`
	`DATABASE NAME /XYN/: <new database name>`

Notes	DATABASE NAME: The new database is specified by typing the abbreviation given in the front of one of the available predefined databases. For convenience when switching/appending databases or recently purchased databases from Thermo-Calc Software or its agents, you can add them to the predefined database list in the database initiation file TC_INITD.TDB or initd.tdb of your installed software.

Syntax	SWITCH_DATABASE
	When this command is used in a MACRO (*.TCM) file, if the USER option is selected, the database setup file name (*setup.TDB) containing the setup definitions of the USER database, and its correct path, must be provided. If a USER database name or its path is not given on the same line of the SWITCH_DATABASE command, or if it is incomplete or incorrect, an Open window displays to specify the filename of the database setup file name (*setup.TDB) of the to-be-switched USER database. Unlike in the DATA module, if a USER database is used, the Gibbs energy system is also reinitialized and only data from the USER databases are retrieved for tabulations. After this command, those commands to define systems (in terms of either elements or species), to reject/restore phases or species, retrieve data, as well as to append data from additional database(s), can be done.

TABULATE

Gives the values of an already-defined table (with various properties varied with the stepping axis variable) from equilibria calculated with a STEP command. You can tabulate a table even if the table is entered after the STEP calculation.

Syntax	TABULATE
Prompts	`NAME: <NAME OF A DEFINED TABLE>` The name of the table must be given. The table must be ENTERED.
	`OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME>` The table can be listed on the screen (by pressing <Enter>), on a file (the file name must be specified here).

TABULATE_DERIVATIVES

This command is mainly for system debugging purposes and for experienced users. It automatically calculates all partial derivatives for a pure phase or solution phase at a given composition.

This is not the same as the chemical potential.

Before using this command, the system must be defined and thermodynamic data retrieved from an appropriate solution database in the DATA module. The phase name can be given in either upper, lower or mixed cases, and can be abbreviated until it is unique, e.g. fcc, BCC, cem, Liq, etc. as the SSOL database is used for the tabulations, or GAS, FE-S, wustite, Fe2O3-hem, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, thermodynamic properties can be tabulated for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Syntax	TABULATE_DERIVATIVES

Prompts

`PHASE NAME /XXXX/: <NAME OF THE PHASE>`

Specify the phase name of a pure phase or a solution phase.

`XXXX` is the last phase the TAB module accounted for. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase.

For a pure phase (such as `Fe-S`, `Wustite`, and `Fe2O3-Hematite`), no further composition definition is needed. For a solution phase with one sublattice (such as `AQUEOUS` solution, `GAS` mixture and `SLAG` solution), it requests *n*-1 site-fraction inputs for the phase constituents (if there are *n* species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the *n*th species is automatically assigned as the rest.

> The sum of input site fractions must not exceed unity.

Example

For example, these prompts and inputs can be seen for a `LIQUID` solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted `Ni` species are assigned as the rest):

```
FRACTION OF CONSTITUENT (RETURN FOR PROMPT): <RETURN> C /1/: .05
CR /1/: .1
FE /1/: < RETURN>
SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER
FE /1/: .8
N /1/: .005
```

For a solution phase with two or more sublattices (such as FCC alloy solution, and ION_

Syntax	TABULATE_DERIVATIVES

	LIQ ionic liquid solution), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (of course, this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice n-1 times if there are n species on such a sublattice in the defined phase; the nth species on each of the sublattices is automatically assigned as the rest. For example, the following prompts and inputs can be seen for an FCC solution phase (from the SSOL5 database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted O species on its sublattice 1 and VA on its sublattice 2 are assigned as the rest):
	`SPECIFY SUBLATTICE (0 FOR ALL) /0/: <RETURN>`
	`FRACTIONS IN SUBLATTICE 1`
	`CR /1/: .1`
	`FE /1/: .8`
	`NI /1/: .0995`
	`FRACTIONS IN SUBLATTICE 2`
	`C /1/: .05`
	`N /1/: .05`

	`TEMPERATURE /2000/: <TEMPERATURE OF INTEREST, IN K>` Specify the temperature of interest in K.
	`PRESSURE /100000/: <PRESSURE OF INTEREST, IN PA>` Specify the pressure of interest in Pa.

Example Output

For the FCC phase in the Fe-Cr-Ni-C-N-O system (using the SSOL database), the following table is obtained at a specified composition:

```
TAB: TAB_DER

Phase name /BCC/: FCC

SPECIFY SUBLATTICE (0 FOR ALL) /0/: <Enter>

FRACTIONS IN SUBLATTICE 1

CR /1/: .1

FE /1/: .8

NI /1/: .3

SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER
```

```
NI /0/: .0995

FRACTIONS IN SUBLATTICE 2

C /1/: .05

N /1/: .05

Temperature /1800/: <Enter>

Pressure /100000/: <Enter>

Gibbs energy: .................... -1.27432533E+05

Helmholz energy: ................. -1.27433205E+05

Enthalpy: ........................  5.95773994E+04

Internal energy: .................  5.95767279E+04

Entropy: .........................  1.03894407E+02

Molar volume: ....................  6.71473258E-06

Thermal expansivity: .............  7.63886416E-05

Isothermal compressibility: .......  6.02925387E-12

Heat capacity at constant pressure:  4.33555074E+01

First partial derivative with respect to CR in sublattice  1     of Gibbs energy:
................ -1.26034739E+05     of enthalpy: ...................  4.63000206E+04
of entropy: ....................  9.57415334E+01     of volume:
.....................  6.87203263E-06

Second partial derivative of Gibbs energy with respect to also

  CR                    in  1:  1.54392858E+05

  FE                    in  1: -1.53353158E+04

  NI                    in  1: -1.71750366E+04

  O                     in  1:  0.00000000E+00

  C                     in  2: -1.82016870E+05

in  2: -3.73062665E+05

  VA                    in  2: -9.36260878E+04

irst partial derivative with respect to FE in sublattice  1     of Gibbs energy:
................ -1.02869265E+05

    of enthalpy: ...................  6.11738912E+04     of entropy:
....................  9.11350866E+01     of volume: .....................
7.53441165E-06

Second partial derivative of Gibbs energy with respect to also

FE                    in  1:  1.82508696E+04

NI                    in  1: -3.07043434E+03

in  1:  0.00000000E+00

C                     in  2: -1.36027071E+05

in  2: -2.13007485E+05
```

```
VA                       in  2: -1.11741180E+05

First partial derivative with respect to NI in sublattice  1     of Gibbs energy:
............... -1.32427029E+05     of enthalpy: ...................  5.21563580E+04
of entropy: ....................  1.02546326E+02     of volume:
.....................  0.00000000E+00

    Second partial derivative of Gibbs energy with respect to also

  NI                       in  1:  1.48390257E+05

in  1:  0.00000000E+00

  C                        in  2: -7.70620431E+04

in  2: -1.61551726E+05

VA                       in  2: -1.12772206E+05

First partial derivative with respect to O in sublattice  1     of Gibbs energy:
............... -2.62929308E+05     of enthalpy: ...................  5.02555370E+04
of entropy: ....................  1.73991581E+02     of volume:
.....................  0.00000000E+00

Second partial derivative of Gibbs energy with respect to also

in  1:  2.99322360E+07

C                        in  2:  0.00000000E+00

N                        in  2:  0.00000000E+00

VA                       in  2: -1.82377137E+05

First partial derivative with respect to C in sublattice  2     of Gibbs energy:
............... -1.59508417E+05     of enthalpy: ...................  1.21269096E+05
of entropy: ....................  1.55987507E+02     of volume:
.....................  1.06885187E-05

Second partial derivative of Gibbs energy with respect to also

C                        in  2:  2.99322360E+05

N                        in  2: -1.90144000E+04

VA                       in  2: -2.78465070E+04

First partial derivative with respect to N in sublattice  2     of Gibbs energy:
............... -2.39671400E+05     of enthalpy: ...................  4.04456947E+04
of entropy: ....................  1.55620608E+02     of volume:
.....................  0.00000000E+00

Second partial derivative of Gibbs energy with respect to also

N                        in  2:  2.99322360E+05

VA                       in  2: -3.30383665E+04

First partial derivative with respect to VA in sublattice  2     of Gibbs energy:
............... -9.52042686E+04     of enthalpy: ...................  5.37142294E+04
of entropy: ....................  8.27324989E+01     of volume:
.....................  6.86700739E-06

Second partial derivative of Gibbs energy with respect to also

VA                       in  2:  1.66290200E+04
```

TABULATE_REACTION

Tabulate thermodynamic property changes for a chemical reaction as a table, or variation of one chosen property can be plotted against temperature as a graph, or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB5 database (by default), or the current database set by the SWITCH_DATABASE command (thus there is no need to use the DATA module before this command). You can select any other database by using *SWITCH_DATABASE* on page 253 in the TAB module.

It is important to remember the rules to specify a reaction:

- The reaction is specified, by giving the reactants and products, such as `Ga+S=GaS`, `5Al+2Fe=Al5Fe2`.
- Under Linux environments, the notation for a chemical formula treats upper and lower cases as the same (such as `ga+s=GaS, 5Al+2Fe=al5fe2`); but under Windows, the TAB module only accepts upper cases, e.g. `GA+S=GAS, 5AL+2FE=AL5FE2`.
- Elements with a single letter symbol must be followed by a stoichiometry factor, even if it is 1; thus, the symbol `CO` is taken as cobalt, carbon monoxide must be given as `C1O1` (or `O1C1`).
- All the reactants and products must be defined as species-stoichiometries in the currently-used database; in other words, the reaction definition only accepts already-defined species-stoichiometries as reactants and products. For example, if a database does not have a species defined with a stoichiometry of Al5Fe2 {e.g. the Al and Fe (but not Al5Fe2) may be defined as species, and the Al5Fe2 phase may be defined as a two-sublattice stoichiometric phase [Al]5[Fe]2, rather than a single sublattice stoichiometric phase [Al5Fe2]}, then the reaction 5Al+2Fe=Al5Fe2 cannot be tabulated.
- Make sure that the Gibbs free energy expression for a stoichiometric phase is really corresponding to the species-stoichiometry. For example, if a database has a definition of Function GAL5FE2 for 1/7 of the AL5FE2 formula, then the relation G(Al5Fe2)-)=7*GAL5FE2 must be defined; otherwise, the tabulated thermodynamic properties for the reaction 5Al+2Fe=Al5Fe2 is wrong.

Syntax	TABULATE_REACTION
Prompts	`SAME REACTION? /Y/: <Y OR N>` This prompt displays if there is at least one reaction already defined either with the commands *ENTER_REACTION* on page 249 or TABULATE_REACTION. If you answer `Y`, then the next prompt is not asked.
	`REACTION: <CHEMICAL REACTION EQUATION> & <RA+RB=PC+PD>` A long reaction can be typed over several lines. A reaction should be terminated by a

Syntax	TABULATE_REACTION

	semicolon (;) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.
	`Pressure /100000/: <pressure of interest, in pa>`
	`Low temperature limit /298.15/: <T-low, in K> Specify the starting temperature K.`
	`High temperature limit /298.15/: <T-high, in K> Specify the ending temperature K. Step in temperature /100/: <T-step> Specify the temperature step for the tabulation.`

	`OUTPUT FILE /SCREEN/: <RETURN FOR SCREEN, OR TYPE A FILE NAME>` If you type `Return for screen`, a list of thermodynamic property changes for the defined/chosen reaction is shown as a table (which is demonstrated in the example outputs given below), and the command is terminated. If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program prompts:
	`GRAPHICAL OUTPUT /Y/: <Y OR N>` • For N a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. • For `Y` a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also asks which column is to be plotted on the resulting graph:
	`PLOT COLUMN? /2/: <1 OR 2 OR 3 OR 4 OR 5 OR 6>` Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST: prompt always takes you back to the TAB module.

Syntax	TABULATE_REACTION
	Also see the *DATPLOT User Guide* included with this documentation set.

Example Output

For the reaction Ga+S=GaS (using the SSUB5 database), the following table is obtained by typing <Enter> in the prompt Output file /SCREEN/, and the figure by typing `2` in the prompt `Plot column /2/`:

```
    O U T P U T   F R O M   T H E R M O - C A L C

     Reaction:  S+GA=GA1S1

 stable as S_S

 GA stable as GA_S

 GA1S1 stable as GA1S1_S

 Delta-Cp      Delta-H       Delta-S       Delta-G

 (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)

 ***************************************************************

 298.15  -2.79489E+00  -2.09200E+05  -1.50580E+01  -2.04710E+05

 300.00  -2.87516E+00  -2.09205E+05  -1.50755E+01  -2.04683E+05

 302.   ---- GA becomes GA_L ,delta-H =   5589.80

 367.   ---- S becomes S_S2 ,delta-H =   401.00

 389.   ---- S becomes S_L ,delta-H =   1721.00

 400.00  -1.22278E+01  -2.17521E+05  -4.07488E+01  -2.01222E+05

 500.00  -1.57686E+01  -2.19323E+05  -4.47280E+01  -1.96959E+05

 600.00  -1.02518E+01  -2.20583E+05  -4.70410E+01  -1.92359E+05

 700.00  -6.58954E+00  -2.21430E+05  -4.83534E+01  -1.87583E+05

 800.00  -4.46246E+00  -2.21963E+05  -4.90686E+01  -1.82709E+05

 900.00  -2.82671E+00  -2.22328E+05  -4.94995E+01  -1.77778E+05

 1000.00  -1.21787E+00  -2.22530E+05  -4.97138E+01  -1.72816E+05

 1100.00   3.71702E-01  -2.22572E+05  -4.97552E+01  -1.67841E+05
```

TABULATE_SUBSTANCE

Tabulate thermodynamic properties of a substance (with a given chemical formula but it is not certain in which phase/state it may form) or a pure stoichiometric phase (getting data from a specific substance database such as SSUB5, or from a specific solution database such as SSOL5 and TCFE8), or of a solution phase with a fixed composition (getting data from a specific solution database such as SSOL5 and TCFE8), under a constant pressure and various temperatures.

In case of a pure stoichiometric phase or a solution phase with a fixed composition, you must already define the system and get thermodynamic data from an appropriate solution database in the DATA module before using this TAB command. The phase name can be given either upper or lower or mixed cases, and can be abbreviated until it is unique, e.g. `fcc`, `BCC`, `Liq`, `cem`, `Al5Fe2`, etc. as the SSOL database is used for the tabulations, or `GAS`, `FE-S`, `wustite`, `Fe2O3-hem`, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, you can tabulate thermodynamic properties for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Moreover, the variation for one of the tabulated properties for a substance, a pure stoichiometric phase, or a solution phase with a fixed composition can be plotted against temperature as a graph or saved as an experimental file (with an extension of .EXP).

Syntax	TABULATE_SUBSTANCE
Prompt	`SUBSTANCE (PHASE): <NAME OF THE SPECIES OR PHASE>` In case of a substance, give its chemical formula, e.g. Fe, H2, C1H6, FeC1, CaC1O3, MgSiO3, etc. When the TABULATE_SUBSTANCE <SUBSTANCE> command sequence is used for the first time in the TAB module, it always uses the SSUB Substances Database as the default database. If the SSUB database is not available for the current Thermo-Calc installation and a specific database has not been switched on yet, it may prompt to specify an appropriate substance or solution database (e.g. typing `SSUB2`, `SSUB3`, `SSUB4`, `SSUB5`; `SSOL2`, `SSOL4`, `SSOL5`; `TCFE3`, `TCFE4`, `TCFE5`, `TCFE6`, `TCFE7`, `TCFE8` etc.). Prior to this command, you can also use the *SWITCH_DATABASE* on page 253 command in the TAB module to set the current database. If a solution database is set as the current database, only the neutral species that are valid substance standing by themselves as phases can be tabulated. Before other prompts, a list of the used database, defined elements, getting-data sequence, references, etc. is displayed on screen. From such information, you know what the TAB module is performing. In case of a pure stoichiometric phase or a solution phase, give its phase name, e.g. FCC, CEMENTITE, LIQUID, SLAG, AQUEOUS, GAS, Al5Fe2, Fe-S, Wustite, Fe2O3-Hematite, etc. REMEMBER: It is important that you have already defined the system and gotten thermodynamic data from an appropriate solution database in the DATA module before using this TAB_SUB command. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase. For a pure stoichiometric phase defined with one single sublattice (such as Fe-S, Wustite, and Fe2O3-Hematite), no further composition definition is needed. For a solution phase defined with one sublattice (such as AQUEOUS solution, GAS mixture and SLAG solution), it requests n-1 site-fraction inputs for the phase constituents (if there are *n* species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the *n*th species is automatically assigned as the rest.

Syntax	TABULATE_SUBSTANCE
	ⓘ The sum of input site fractions must not exceed unity. For example, the following prompts and inputs can be seen for a LIQUID solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted Ni species is assigned as the rest):

```
FRACTION OF CONSTITUENT (RETURN FOR PROMPT): <RETURN>
  C /1/: .05
  CR /1/: .1
  FE /1/: <RETURN>
```

```
SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER
  FE /1/: .8
  N /1/: .005
```

For a pure stoichiometric phase defined with two or more sublattices (such as Al5Fe2 intermetallic stoichiometric phase) and for a solution phase defined with two or more sublattices (such as FCC alloy solution, and ION_LIQ ionic liquid solution, Al5Fe4 intermetallic solution phase), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice *n*-1 times if there are n species on such a sublattice in the defined phase; the *n*th species on each of the sublattices are automatically assigned as the rest. For example, these prompts and inputs can be seen for an FCC solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted `O` species on its sublattice `1` and `VA` on its sublattice `2` is assigned as the rest):

```
SPECIFY SUBLATTICE (0 FOR ALL) /0/: <RETURN>
  FRACTIONS IN SUBLATTICE            1
  CR /1/: .1
  FE /1/: .8
  NI /1/: .0995
  FRACTIONS IN SUBLATTICE            2
  C /1/: .05
  N /1/: .05
```

Syntax	TABULATE_SUBSTANCE
	`PRESSURE /100000/: <PRESSURE OF INTEREST, IN PA>` Specify the constant pressure condition in Pa.
	`LOW TEMPERATURE LIMIT /298.15/: <T-LOW, IN K>` Specify the starting temperature K.
	`HIGH TEMPERATURE LIMIT /298.15/: <T-HIGH, IN K>` Specify the ending temperature K.
	`STEP IN TEMPERATURE /100/: <T-STEP> SPECIFY THE TEMPERATURE STEP FOR THE TABULATION.`
	`OUTPUT FILE /SCREEN/: <RETURN FOR SCREEN, OR TYPE A FILE NAME>` If you type `Return for screen` a list of basic thermodynamic functions for the chosen substance or for the specified pure or solution phase with the fixed composition is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated. If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program further prompts:
	`GRAPHICAL OUTPUT /Y/: <Y OR N>` • For `N` a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. • For `Y` a table is created with all the thermodynamic functions as normal (which is displayed on screen) as well as generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also ask which column is to be plotted on the resulting graph:
	`PLOT COLUMN ? /2/: <1 OR 2 OR 3 OR 4 OR 5 OR 6>` Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-

Syntax	TABULATE_SUBSTANCE
	axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST: prompt always takes you back to the TAB module.
	Also see the *DATPLOT User Guide* included with this documentation set.

Example Output 1

For the `FCC` alloy phase as a non-ideal solution with a fixed composition

```
[Fe0.80,Cr0.10,Ni0.0995,O0.005][C0.05,N0.05,VA0.90]
```

The following table is obtained by typing `Return for screen` at the prompt `Output file /SCREEN/`:

```
O U T P U T   F R O M   T H E R M O - C A L C

Phase : FCC                         Pressure :      100000.00

Specie: CR1/--2

***************************************************************

    T       Cp             H             S             G

   (K)     (Joule/K)      (Joule)       (Joule/K)      (Joule)

***************************************************************

298.15    2.70517E+01   6.23824E+03   4.40241E+01  -6.88755E+03

300.00    2.70889E+01   6.28832E+03   4.41916E+01  -6.96915E+03

400.00    2.87304E+01   9.08420E+03   5.22235E+01  -1.18052E+04

500.00    2.99904E+01   1.20222E+04   5.87742E+01  -1.73649E+04

600.00    3.10889E+01   1.50770E+04   6.43408E+01  -2.35275E+04

700.00    3.21116E+01   1.82375E+04   6.92106E+01  -3.02100E+04

800.00    3.30994E+01   2.14982E+04   7.35633E+01  -3.73524E+04

900.00    3.40742E+01   2.48569E+04   7.75182E+01  -4.49094E+04

1000.00    3.50483E+01   2.83130E+04   8.11586E+01  -5.28456E+04

1100.00    3.60268E+01   3.18667E+04   8.45449E+01  -6.11327E+04

1200.00    3.70143E+01   3.55187E+04   8.77219E+01  -6.97476E+04

1300.00    3.80149E+01   3.92700E+04   9.07241E+01  -7.86713E+04

1400.00    3.90311E+01   4.31222E+04   9.35784E+01  -8.78875E+04

1500.00    4.00649E+01   4.70768E+04   9.63064E+01  -9.73827E+04

1600.00    4.11174E+01   5.11358E+04   9.89256E+01  -1.07145E+05

1700.00    4.21896E+01   5.53010E+04   1.01450E+02  -1.17165E+05

1800.00    4.33555E+01   5.95774E+04   1.03894E+02  -1.27433E+05
```

```
1900.00    4.58528E+01    6.40379E+04    1.06306E+02   -1.37943E+05

2000.00    4.75402E+01    6.87138E+04    1.08704E+02   -1.48694E+05
```

Example Output 2

For a phase, as either an end-member or real solution, the listed species name is irrelevant.

For the H2 species as a pure substance (using the SSUB5 database), the following table is obtained by typing `Return for screen` at the prompt `Output file /SCREEN/`, whilst the figure is generated by typing 5 at the prompt Plot column /2/:

```
            O U T P U T F R O M T H E R M O - C A L C

     Phase : GAS                                Pressure :      100000.00

  Specie: H2

  ***************************************************************     T       Cp
  H              S              G

     (K)     (Joule/K)       (Joule)       (Joule/K)       (Joule)

  ***************************************************************   298.15    2.88369E+01
  3.17684E-06    1.30680E+02   -3.89622E+04

  300.00    2.88473E+01    5.33580E+01    1.30858E+02   -3.92042E+04

  400.00    2.91591E+01    2.95686E+03    1.39209E+02   -5.27268E+04

  500.00    2.92650E+01    5.87874E+03    1.45729E+02   -6.69856E+04

  600.00    2.93441E+01    8.80908E+03    1.51071E+02   -8.18336E+04

  700.00    2.94579E+01    1.17488E+04    1.55602E+02   -9.71730E+04

  800.00    2.96320E+01    1.47027E+04    1.59547E+02   -1.12935E+05

  900.00    2.98786E+01    1.76776E+04    1.63050E+02   -1.29068E+05

  1000.00    3.02043E+01    2.06810E+04    1.66214E+02   -1.45533E+05

  1100.00    3.05319E+01    2.37171E+04    1.69108E+02   -1.62302E+05

  1200.00    3.09281E+01    2.67897E+04    1.71781E+02   -1.79348E+05

  1300.00    3.13615E+01    2.99040E+04    1.74274E+02   -1.96652E+05

  1400.00    3.18115E+01    3.30625E+04    1.76614E+02   -2.14197E+05

  1500.00    3.22641E+01    3.62664E+04    1.78824E+02   -2.31970E+05

  1600.00    3.27094E+01    3.95151E+04    1.80921E+02   -2.49958E+05

  1700.00    3.31406E+01    4.28078E+04    1.82917E+02   -2.68151E+05

  1800.00    3.35526E+01    4.61426E+04    1.84823E+02   -2.86539E+05

  1900.00    3.39415E+01    4.95175E+04    1.86648E+02   -3.05113E+05

  2000.00    3.43045E+01    5.29300E+04    1.88398E+02   -3.23866E+05
```

TERNARY_DIAGRAM Commands

In this section:

TERNARY_DIAGRAM Module

The TERNARY_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple ternary phase diagram.

To enter the module, at the SYS prompt type GOTO_MODULE TERNARY. There are no other commands for this module. Follow the prompts to plot a diagram.

Also see the Graphical Mode equivalent to this command, *Ternary Calculator* on page 107 as described in the *Thermo-Calc User Guide*.

Syntax	TERNARY_DIAGRAM
Prompts	`DATABASE: /FEDEMO/`

	`FIRST ELEMENT:`
	`SECOND ELEMENT`
	`THIRD ELEMENT`

	`PHASE DIAGRAM, MONOVARIANTS, OR LIQUIDUS SURFACE: /PHASE_DIAGRAM/`
	`TEMPERATURE (C) /1000/`
	`GLOBAL MINIMIZATION ON: /Y/`

Thermodynamic Variables and Units

The following topics are about the different thermodynamic variables recognised by Thermo-Calc. The topics have information about how to define new derived variables and functions and how to express thermodynamic variables in non-default units. The POLY module only recognises default units, which are the SI units.

See example 44 Thermo-Calc Console Mode Examples to learn about using variables and functions.

In this section:

Thermodynamic Variables

There are different thermodynamic variables in Thermo-Calc. Some are *state variables*, for example temperature, pressure and mole fraction. These characterize the equilibrium state of a system. You set them when you define your system in the POLY module before performing a calculation. They are also used in other modules such as DATA, GIBBS and PARROT. State variables that involve components can be used for the defined components, but not for any species. (To define new components in a defined system, use *DEFINE_COMPONENTS* on page 143).

Other useful thermodynamic variables are derive from state variables with a mathematical function. Some derived variables are pre-defined by Thermo-Calc, such as normalized energetic and compositional extensive state variables for example. You use these by appending various normalizing suffixes to abbreviations that are associated with the state variables.

Thermodynamic variables can also be divided into extensive variables and intensive variables. An extensive variable is a variable whose value depends on the size of the system, whereas an intensive variable is a variable whose value is independent of system size.

More information about thermodynamic variables is available in the online help in Thermo-Calc Console Mode. Use the command *INFORMATION* on page 5, with a subject keyword such as one of the following as argument: STATE VARIABLES, INTENSIVE VARIABLES, EXTENSIVE VARIABLES, DERIVED VARIABLES, CONDITIONS (for condition settings), AXIS-VARIABLES (for stepping/mapping variable settings).

Common Thermodynamic Variables

The tables below list common thermodynamic variables. Most of these can be used to define equilibrium conditions in the POLY module unless otherwise indicated.

The variables are divided into the following tables:

- Intensive variables
- Energy-related extensive variables for whole system or for a phase
- Compositional extensive variables (overall amount of components in the whole system, or amount of a component in system or in a phase)
- Constitutional composition-related extensive variables (amount of a constituent/species on a sublattice site in a phase)
- Special quantities

How to Read the Tables

- The *Abbrev*. column shows the abbreviation that you use in the POLY module for referring to the variable. If the variable must be given any arguments, then these are given in parenthesis directly after the abbreviation. For most variables, this is also the abbreviation that you use to refer to the variable in other modules. However, some variables are referred to with a different abbreviation in the POST module. If this is the case, then this is noted at the bottom of the table.

- Variables that are specific to a species, in which case the species is specified as an argument (*sp* in the table below). If there are two or more sublattices in a given phase, then this argument is given as `constituent#sublattice`. This indicates a constituent on a specific sublattice or site in the phase (referred to by the # sign and a digit). For example, `y(BCC,C#2)` stands for the site fraction of the C species on the second sublattice site of the BCC_A2 solution phase.
- The *Unit* column show which unit that you can use to express the variable in the POLY module. This unit is always the SI unit. In other modules, state variables may be expressed in other units.
- The *Suffix* column shows the suffixes you can append to the variables. The R-suffix can be used with all compositional extensive state variables, but the suffix does not always change the value of the variable. This is indicated by putting the `R` in parenthesis.

These types of variables are listed in the following topics:

- *Intensive Variables* below
- *Extensive Variables* on the next page
- *Special Quantities* on page 277
- *The u-Fraction Variable* on page 278
- *Suffixes* on page 278

Intensive Variables

V	Abbrev.	Unit	Descript.	Domain	Suffix
T	T[1]	K	Temperature	System	
P	P	Pa	Pressure	System	
μ	MU(comp)	J/mol	Chemical potential	Component	R
	MU(sp,ph)[2]			Species relative to a solution phase	R

V	Abbrev.	Unit	Descript.	Domain	Suffix
a	AC(comp)	N/A	Activity	Component	R
	AC(sp,ph)[2]			Species relative to a solution phase	R
	LNAC (comp)[3]		ln(Activity)	Component	R
	LNAC (sp,ph) [2]			Species relative to a solution phase	R

[1] When plotting in POST, besides T (Kelvin), you can also use T_C or T_F to plot temperature in °C or °F.

[2] Only for single-substitutional-lattice solution phases such as AQUEOUS solution and GASeous mixture phases and for interacting species on the substitutional sublattice of two-sublattice solution phases (such as the phases BCC_A2 and M6C phases).

[3] In natural logarithm (lnAC=MU/RT)

Extensive Variables

Energy-Related Extensive Variables for Whole System or for a Phase

See example 44 in the *Console Mode Examples Guide*for an example of using variables and functions.

V	Abbrev.	Unit	Descript.	Domain	Suffix
V	V	m3	Volume	System	M, W, V, R
	V(ph)[1]			Phase	M, W, F, R
	VP(ph) [2]			Phase	M, W, V, R
G	G	J	Gibbs energy	System	M, W, V, R
	G(ph) [1]			Phase	M, W, V, F, R
A	A	J	Helmholtz energy	System	M, W, V, R
	A(ph) [1]			Phase	M, W, V, F, R

V	Abbrev.	Unit	Descript.	Domain	Suffix
U	U	J	Internal energy	System	M, W, V, R
	U(ph)[1]			Phase	M, W, V, F, R
H	H	J	Enthalpy	System	M, W, V, R
	H(ph)			Phase	M, W, V, F
S	S	J/K	Entropy	System	M, W, V, R
	S(ph)[1]			Phase	M, W, V, F, R
Cp	HM.T[3]	J/mol/K	Heat capacity at constant pressure	System	R
	HM(ph).T[3]			Phase	R
Cv	HM.T[4]	J/mol/K	Heat capacity at constant volume	System	R
	HM(ph).T[4]			Phase	R
D	DG(ph)[5]	N/A	Driving force (thermodynamic factor)	Phase	Always use with M, W, V or F. R can also be used.

[1] For this variable, if the phase is unstable, then the variable gets a value of zero.

[2] Do not use VP(ph) as a condition in POLY. Instead, use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to VPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then VP(ph) and its normalized quantities get zero value.

[3] Use only if pressure has been set as a condition.

[4] Use only if volume has been set as a condition.

[5] Already divided by RT.

Compositional Extensive Variables

These are for the overall amount of components in whole system, or amount of a component in system or in a phase.

Do not use NP(ph) or BP(ph) as conditions in the POLY module. Instead use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to NPF(ph) or BPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then NP(ph) or BP(ph) (and its normalized quantities) get zero value.

When plotting the following quantities in POST, refer to each as indicated:

- X(comp) -> `Mole-Fraction <comp>` (or `M_F`)
- W(comp) -> `Weight-Fraction <comp>` (or `W_F`)
- X%(comp) -> `Mole-Percent <comp>` (or `M_P`)
- W%(comp) -> `Weight-Percent <comp>` (or `W_P`).
- u-f(ph,comp) -> `U-F`

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
n	N	mole	Moles	All components	M, W, V, (R)	
	N(comp)			Component	M, W, V, (R)	
	N(ph,comp)			Component in a phase	M, W, V, (R)	
	NP(ph)[1]			Phase	M, W, V, (R)	See above
b	B	gram	Mass	All components	M, W, V, (R)	
	B(comp)			Component	M, W, V, (R)	
	B(ph,comp)			Component in a phase	M, W, V, (R)	
	BP(ph) [1]			Phase	M, W, V, (R)	See above
x	X(comp)	N/A	Mole fraction	Component	(R)	See above
	X(ph,comp)			Component in a phase	(R)	
w	W(comp)	N/A	Mass (weight) fraction	Component	(R)	See above
	W(ph,comp)			Component in a phase	(R)	
x%	X%(comp)[2]	N/A	Mole percent	Component	(R)	See above
w%	W%(comp)[2]	N/A	Mass (weight) percent	Component	(R)	See above
u	u-f (ph,comp)[1]	N/A	u-fraction	Component in a stable phase	(R)	See above

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
in	IN(sp)[2]	mole	Input mole number	Phase species in the system	(R)	See above
im	IM(sp)[2]	gram	Input mass unit	Phase species in the system	(R)	See above

[1] Do not use as a condition in the POLY module.

[2] Only available in TQ-Interface and TC-API.

Constitutional Composition-Related Extensive Variable

This is the amount of a constituent/species on a sublattice site in a phase.

V	Abbrev.	Unit	Descript.	Domain
y	Y (ph,cons#sub)	N/A	Site fraction	Constituent on a sublattice site (denoted by # and a digit) in a phase

Special Quantities

V	Abbrev.	Unit	Descript.	Domain	Suffix
Q	QF(ph)[1]	N/A	Phase stability function	Phase	R Under a condition and system definition, QFR (ph) = QF(ph)
Tc	TC(ph) [2]	K	Curie temperature	Phase	R Under a condition and system definition, TCR (ph) = TC(ph)
Mb	BMAG(ph)[3]	N/A	Bohr magneton number	Phase	R Under a condition and system definition, BMAGR (ph) = BMAG(ph)

[1] Negative when phase composition is inside a spinodal, otherwise positive. Can be used to find out if an equilibrium is within the miscibility gap for a solution phase. Cannot be used as a condition.

[2] Calculated for phases with magnetic contributions in an equilibrium state. Cannot be used as a condition, but can be plotted in POST or evaluated in POLY using *SHOW_VALUE* on page 172.

V	Abbrev.	Unit	Descript.	Domain	Suffix
[3] Calculated for phases with magnetic contributions in an equilibrium state.					

The u-Fraction Variable

The u-fraction is an important quantity in some single-point or stepping paraequilibrium calculations in the POLY module and in the DICTRA module. You can apply the variable in a paraequilibrium calculation to the substitutional matrix component, the substitutional alloying components or the interstitial component. The u-fraction is denoted as ui for the i-th system component *n* of a whole system or of a specific phase in various equilibrium states (such as full-equilibria, partial-equilibria, para-equilibria, local-equilibria).

Generally, the u-fraction is defined as:

$$\frac{x_i}{\sum_{j \in S} x_j}$$

The sum of *x*j in the denominator is calculated for all substitutional alloying elements in the whole system or in a specific phase. The variable x_i in the numerator stands for the mole-fraction of the *i*-th component in the whole system or in the specific phase.

Suffixes

Suffixes may be appended to all extensive variables and to some intensive variables. Some suffixes can be used to enter the value of variables in normalized form. These are referred to as normalizing suffixes. If the variable that you create with a normalizing suffix is based on a state variable that can be set as a condition in POLY, then the normalized variable can also be set as a condition in POLY.

The normalizing suffixes are M (per mole), W (per mass in gram), V (per volume in m^3) and F (per mole formula unit). There is also a reference state suffix `R`, which you can use if you want the value of a thermodynamic variable to be calculated with respect to a reference state that have previously set.

Normalizing Suffixes

When variables that express system and phase quantities are normalized, the following general rules are used:

- System quantities are normalized by the total system size (in terms of N, B or V).
- Phase quantities are normalized by the phase amount [in terms of NP(ph), BP(ph) or VP (ph)].

The normalized quantities of G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) are calculated according to the thermodynamic model used for the phase (e.g. GM(ph), AM(ph), UM(ph), HM(ph), SM(ph) and VM(ph)).

These quantities are calculated using the first derivatives of the Gibbs energy expressed for the phase with respect to the current composition of the system.

The tables describe the normalizing suffixes for the different state variables.

G, A, U, H, S and V of a Whole System

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the total system size in terms of N.	GM is the Gibbs energy per mole of the system (J/mol). GM = ∂G/∂N
W (per mass in gram)	First derivative of the variable with regard to the total system size in terms of B.	GW is the Gibbs energy per mass of the system (J/g). GW = ∂G/∂B
V (per volume in m^3)	First derivative of the variable with regard to the total system size in terms of V. VV does not have to be evaluated.	GV is the Gibbs energy per volume of the system (J/m3). GV = ∂G/∂V

G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) of a Phase

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the phase amount in terms of NP(ph).	GM(ph) is Gibbs energy of the phase per mole of the phase (J/mol). GM(ph) = ∂G(ph)/∂NP(ph)
W (per mass in gram)	First derivative of the variable with regard to the phase amount in terms of BP(ph).	GW(ph) is Gibbs energy of the phase per mass of the phase (J/mol). GW(ph) = ∂G(ph)/ ∂BP(ph)
V (per volume in m^3)	First derivative of the variable with regard to the phase amount in terms of VP(ph). VV(ph) does not have to be evaluated.	GV(ph) is Gibbs energy of the phase per volume of the phase (J/mol). GV(ph) = ∂G(ph)/∂VP(ph)
F (per mole formula unit)	First derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula)	GF(ph) is the Gibbs energy of the phase per formula unit of the phase (J/mol). GF(ph) = ∂G(ph)/∂NP(ph)*NA

DG(ph) of a Phase

Suffix	Description	Example(s)
M (per mole)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph). Since DG (ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGM(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGM(ph) is driving force for precipitation of the phase per mole of components. DGM(ph) = ∂DG(ph)/∂NP(ph)
W (per mass in gram)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of BP(ph). Since DG (ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGW(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGW(ph) is driving force for precipitation of the phase per mass of components. DGW(ph) = ∂DG(ph)/∂BP(ph)
V (per volume in m^3)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of VP(ph). Since DG (ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGV(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGV(ph) is driving force for precipitation of the phase per volume of components. DGV(ph) = ∂DG(ph)/∂VP(ph)
F (per mole formula unit)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGF(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGF(ph) is driving force for precipitation of the phase per formula unit of components. DGF(ph) = ∂DG(ph)/∂NP (ph)*NA

N and B of a System

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the total system size in terms of N. NM does not have to be evaluated. BM cannot be set as a condition.	BM is mass (gram) of components per mole of the system (g/mol). BM = ∂B/∂N
W (per mass in gram)	First derivative of the variable with regard to the total system size in terms of B. BW does not have to be evaluated. NW cannot be set as a condition.	NW is mole number of components per mass of the system (mol/g). NW = ∂N/∂B
V (per volume in m^3)	First derivative of the variable with regard to the total system size in terms of V. BV is the density of the entire system.	NV is mole number of components per volume of the system (mol/m^3). NV = ∂N/∂V BV is the density of the entire system (g/m^3). BV = ∂B/∂V

N (comp) and B(comp) of a Component in the System

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the total system size in terms of N. BM(comp) cannot be set as a condition.	NM(comp) is the mole of a component per mole of the system (i.e. mole fraction, which also is expressed as X(comp)). NM(comp) = ∂N(comp)/ ∂N
W (per mass in gram)	First derivative of the variable with regard to the total system size in terms of B. NW(comp) cannot be set as a condition.	BW(comp) is mass (gram) of a component per mass of the system (i.e. mass fraction, which also is expressed as W(comp)). BW(comp) = ∂B(comp)/∂B
V (per volume in m^3)	First derivative of the variable with regard to the total system size in terms of V.	NV(comp) is mole number of a component per volume of the system (mol/m3). NV(comp) = ∂N(comp)/ ∂V

NP(ph), BP(ph) and VP(ph) of a Phase in the System

Suffix	Description	Example(s)
M (per mole)	BPM(ph) and VPM(ph): First derivative of the variable with regard to the phase amount in terms of NP(ph). NPM(ph): First derivative of the variable with regard to the total system size in terms of N.	BPM(ph) is mass (gram) of a phase per moles of the system (g/mol). BPM(ph) = ∂BP(ph)/∂N NPM(ph) is number of moles of a phase per moles of the system (mole fraction). NPM(ph) = ∂NP(ph)/∂N
W (per mass in gram)	NPW(ph) and VPW(ph): First derivative of the variable with regard to the phase amount in terms of BP(ph). BPW(ph): First derivative of the variable with regard to the total system size in terms of B.	VPW(ph) is volume (m3) of a phase per mass of the system (m3/g) VPW(ph) = ∂VP(ph)/∂B BPW(ph) is mass (gram) of a phase per mass of the system (mass fraction) BPW(ph) = ∂BP(ph)/∂B
V (per volume in m^3)	NPV(ph) and BPV(ph): First derivative of the variable with regard to the phase amount in terms of VP(ph). VPV(ph): First derivative of the variable with regard to the total system size in terms of V.	NPV(ph) is number of moles of a phase per volume of the system (mol/m3). NPV(ph) = ∂NP(ph)/∂V VPV(ph) is volume (m3) of a phase per volume of the system (volume fraction). VPV(ph) = ∂VP(ph)/∂V

N(ph,comp) and B(ph,comp) of a Component in a Phase

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the phase amount in terms of NP(ph) of the phase.	NM(ph,comp)is number of moles of a component per mole of a phase (i.e. mole fraction of a component in a phase, which is equivalent to X(ph, comp)). NM(ph,comp) = ∂N(ph,comp)/∂NP(ph)
W (per mass in gram)	First derivative of the variable with regard to the phase amount in terms of BP(ph) of the phase.	BW(ph,comp) is mass (gram) of a component per mass of a phase (i.e. mass fraction of a component in a phase, which is equivalent to W(ph,comp)). BW(ph,comp) = ∂B(ph,comp)/∂BP(ph)

Suffix	Description	Example(s)
V (per volume in m^3)	First derivative of variable with regard to the phase amount in terms of VP(ph) of the phase.	NV(ph,comp) is mole number of a component per volume of a phase (mol/m3). NV(ph,comp) = ∂N(ph,comp)/∂VP(ph)

The Reference State Suffix R

You can use the reference state suffix `R` for some thermodynamic variables to calculate their value with respect to a reference state that you have previously set for a system component with the *SET_ REFERENCE_STATE* on page 169 command in POLY (or in a response-driven modules such as the POURBAIX module). The value of energy-related variables that are used with the `R` suffix depends on the reference states of all the components in the defined system.

It is possible to use an `R` suffix on all compositional extensive state variables as well, but the value of the state variable is always the same, with or without the suffix.

If the reference state for a system component is the default reference state (the stable reference state (SER) which is defined in a Thermo-Calc database), then MUR(comp)= MU(comp), ACR(comp)= AC(comp) and LNACR(comp)= LNAC(comp).

In the case of some thermodynamic variables, you can also use the `R` suffix to express chemical potentials and activities of species relative to some single-substitutional-lattice solution phases (such as aqueous solution, gaseous mixture, metallic liquid solution, slag mixture or MO solid solution). These state variables are MU(sp,ph), MUR(sp,ph), AC(sp,ph), ACR(sp,ph), LNAC(sp,ph) and LNACR(sp,ph).

The reference states and standard states of various solution species are pre-defined for some solution phases in some databases. For all solution species in any solution model in any database, it is always the case that MUR(sp,ph)= MU(sp,ph), ACR(sp,ph)= AC(sp,ph) and LNACR(sp,ph)= LNAC(sp,ph).

Derived Variables and Partial Derivatives

Many derived variables can be obtained easily by using partial derivatives of state variables, such as heat capacity, thermal expansivity, isothermal compressibility, among others.

Derivatives of state variables can be defined or evaluated by putting a dot (`.`) between two state variables. The variable after the dot must be a condition that you have set when you defined your system. For example, the heat capacity (at constant pressure or volume) of a system is the partial derivative of the state variable enthalpy with respect to temperature. To evaluate this derivative, use the designation HM.T, where temperature is a state variable that you have set already.

Any partial derivative of a state variable with respect to another can be defined or evaluated as a derived variable by using the dot (`.`) notation.

Derived Variables Dot Notation Examples

The following table shows some examples:

Derived variable	Description
HM.T = ∂HM/∂T	Heat capacity for the system at either constant P if pressure is a condition or constant V if volume is a condition.
HM(ph).T = ∂HM(ph)/ ∂T	Heat capacity for a phase at either constant P if pressure is a condition or constant V if volume is a condition.
H.T = ∂H/∂T	Heat capacity for the system multiplied by total mole number of components, i.e., ∂H/∂T = Cp*N if pressure is a condition in a closed system or ∂H/∂T = Cv*N if volume is a condition in a closed system.
H(ph).T = ∂H(ph)/ ∂T	Heat capacity for a phase multiplied by the sum of NP(ph) and HM(ph)*∂NP(ph)/∂T, i.e., Cp(ph)*NP(ph)+HM(ph)*∂NP(ph)/∂T if pressure is a condition or Cv(ph)*NP(ph)+HM(ph)*∂NP (ph)/ ∂T if volume is a condition.
VM.T = ∂VM/∂T	Thermal expansivity of the system (already multiplied by the total molar volume), i.e., ∂VM/∂T = α*VM.
VM(ph).T = ∂VM(ph)/∂T	Thermal expansivity of a phase (already multiplied by its molar volume), i.e., ∂VM(ph)/ ∂T = α(ph)*VM (ph).
V.T = ∂V/∂T	Thermal expansivity of the system (already multiplied by the total volume), i.e., ∂V/∂T = α*V.
V(ph).T = ∂V(ph)/∂T	Thermal expansivity of a phase (already multiplied by the phase volume) plus the VM(ph)*∂NP(ph)/∂T term, i.e., ∂V (ph)/∂T = α(ph)*V(ph)= α(ph)*VM (ph)*NP(ph)+VM (ph)*∂NP (ph)/∂T.
VM.P = -∂VM/∂P	Isothermal compressibility of the system (already multiplied by the total molar volume), i.e., ∂VM/∂P = -κ*VM.
VM(ph).P = -∂VM(ph)/ ∂P	Isothermal compressibility of a phase (already multiplied by its molar volume), i.e., ∂VM(ph)/∂P = -κ(ph)*VM (ph).
V.P = -∂V/∂P	Isothermal compressibility of the system (already multiplied by the total volume), i.e., ∂V/∂P = -κ*V.
V(ph).P = -∂V(ph)/∂P	Isothermal compressibility of a phase (already multiplied by the phase volume) plus the VM(ph)*∂NP(ph)/∂P term, i.e., ∂V (ph)/∂P = -κ(ph)*V(ph) = -κ (ph)*VM (ph)*NP(ph)+VM (ph)*∂NP (ph)/∂P.
T.X(comp) = ∂T/∂X(comp)	Slope of a phase boundary on a T-X(comp) phase diagram with respect to mole fraction of the component in the system.

Derived variable	**Description**
T.W(comp) = ∂T/∂W(comp)	Slope of a phase boundary on a T-W(comp) phase diagram with respect to mass of the component in the system.
T.X(ph,comp) = ∂T/∂X(ph,comp)	Slope of a phase boundary on a T-X(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
T.W(ph,comp) = ∂T/∂W(ph,comp)	Slope of a phase boundary on a T-W(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
P.T = ∂P/∂T	Slope of a phase boundary on a P-T phase diagram (Note that the equilibrium with phase assemblage must be calculated first).

Defining New Derived Variables and Functions

You can define additional derived variables or functions based on a state variable by using *ENTER_SYMBOL* on page 195. Any derived variable or function must have a unique name that starts with a letter and has a maximum number of eight characters. These characters can include both uppercase and lowercase letters, numerical digits and the underscore (_). No other characters are allowed.

The difference between new derived variables introduced with the ENTER_SYMBOL command and new functions introduced with the same command is as follows. Whenever Thermo-Calc calculates the value of a function (as part of an equilibrium calculation for example), all functions related to the defined system is evaluated. An entered derived variable, on the other hand, is only evaluated when it is defined and when it is re-evaluated with *EVALUATE_FUNCTIONS* on page 155.

Derived Variables for Aqueous Solutions

Standard state variables used for other phases can be directly applied to the aqueous solution phase. In addition, there are pre-defined derived variables for the aqueous solution phase in particular.

Examples of predefined derived variables for the aqueous solution phase are listed and briefly described in the following tables. Some derived variables for a gaseous mixture phase are also shown. This is because EOS (Equation of State) expressions, standard thermodynamic properties and transport properties of the pure solvent H2O are also expressions and properties of the pure gaseous species H2O.

For Aqueous Solution Phase

Name	Abbrev.	Units	Description	Comments
pH	PH	N/A	Acidity	of the aqueous solution phase pH = -log10(AC(H+)) = -log10(ACR(H+,AQ))
Eh	EH	V, mV	Hypothetical electric potential	of the aqueous solution phase Eh = u(ZE)/96485.309
Pe	PE	N/A	Logarithm of the hypothetical electron activity	of the aqueous solution phase pe = u(ZE)/(2.3025851*RT)
Ah	AH	kJ, kcal	Thermodynamic affinity per electron	of a redox couple wrt the standard hydrogen electrode in the aqueous solution phase Ah = u(ZE)
yw	YH2O	N/A	Mole fraction	of the solvent H2O in the aqueous solution phase YH2O = Y(AQ,H2O)
Nw	AH2O	mole	Mole number	of 1.0 kg of solvent H2O AH2O = 55.508435
Nsp	NSH2O	mole	Mole number, NS(AQ,H2O)	of the solvent (H2O) in the aqueous solution phase NS(AQ,H2O) = YH2O*NP (AQ)
	NS#		Mole number, NS(AQ,sp)	of a solute species in the aqueous solution phase NS(AQ,sp) = Y(AQ,sp)*NP (AQ)
M	ML#	mol/kg_ H2O	Molality, ML(AQ,sp)	of a solute species in the aqueous phase ML(AQ,sp) = Y (AQ,sp)*AH2O/YH2O

Name	Abbrev.	Units	Description	Comments
m*	TIM	equivalent molality	Total molality	of all solute species in the aqueous solution phase TIM = sum[ML(AQ,sp)]ions + sum[ML (AQ,sp)]complexes
mt	TIC#	equivalent molality	Total ionic concentration, TIC (AQ,sp)	of a cation I in the aqueous phase TIC(AQ,spI) = sum[ML (AQ,spJ)*V(spI-in-spJ)]
I	ISTR	N/A	Ionic strength	of the aqueous solution phase ISTR=1/2*sum[ML (AQ,sp)*Z(AQ,sp)**2]
γ	RCH2O	N/A	Activity coefficient, RC(H2O,AQ)	of the solvent (H2O) RC(H2O,AQ) = ACR (H2O,AQ)/YH2O
	RC#		Activity coefficient, RC(sp,AQ)	of a solute species RC(sp,AQ) = ACR(sp,AQ)/Y (AQ,sp)*YH2O
αi	AIH2O	N/A	Activity, AI(H2O,AQ)	of the solvent (H2O), AI(H2O,AQ) = ACR (H2O,AQ)
	AI#		Activity, AI(sp,AQ)	of a solute species related to the aqueous solution phase, AI(sp,AQ) = ACR (sp,AQ)*AH2O
	LogAI#		Log10 Activity, LogAI (H2O,AQ), LogAI(sp,AQ)	of the solvent or a solute species related to the aqueous solution phase in common logarithm, LogAI(H2O,AQ) = log10 [AI(H2O,AQ)]

Name	Abbrev.	Units	Description	Comments
				LogAI(sp,AQ) = log10[AI (sp,AQ)]
αw	AW	N/A	Activity	of H2O in the aqueous solution phase AW = ACR(H2O,AQ)
ϕ	OS	N/A	Osmotic coefficient	of aqueous solution phase OS = -55.508435*lnAW/TIM
At1	AT1	equil_ mol/kg_ H2O	Titration alkalinity (definition 1)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate at the methyl orange endpoint (pH=4.5).
At2	AT2	equil_ mol/kg_ H2O	Titration alkalinity (definition 2)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate, plus sulfide, at the methyl orange endpoint (pH=4.5).

For Gaseous Mixture Phase

Name	Abbrev.	Units	Description	Comments
γ	RA#	N/A	Activity coefficient, RA(sp,GAS)	of a gaseous species in the gaseous mixture RA(sp,GAS) = function(Y,T,P)
γ^*	RF#	N/A	Fugacity coefficient, RF(sp,GAS)	of a pure gaseous species under TP RF(sp,GAS) = function(T,P/V)
F	FUG#	pa, bar, psi	Fugacity, FUG(sp,GAS)	of a gaseous species in the gaseous mixture FUG(sp,GAS) = RA(sp,GAS)*RF(sp,GAS)*Y (GAS,sp)*P

Name	Abbrev.	Units	Description	Comments
ft	TFUG	pa, bar, psi	Total gas fugacity	of the gaseous mixture phase TFUG = sum[FUG(sp,GAS)]

Defining New Derived Variables for Aqueous Solutions

You can define many different additional derived variables and functions. For instance, the partition coefficient of a component between two phases is defined as follows:

```
Pc<name> = X(phase1,component)/X(phase2,component)
```

Another example is the activity coefficient of a component in the system. It is defined as follows:

```
Rc<name> = ACR(component)/X(component)
```

The activity coefficient of a species in a solution phase depends on which model definitions on the reference states that are used and it depends on the standard states for the species. If the standard state of a species is defined to be the same as the pure species in a substitutional phase, then the activity coefficient of the species can be calculated as:

```
RC<name> = ACR(species,phase)/Y(phase,species)
```

In some cases, there are more than one sublattice in the phase and the reference states for the phase species cannot be presented by the pure species, as in the case of C in FCC [(Fe)1(C,N,VA)1], where the model may end at fifty percent C and fifty percent Fe. In those cases, the chemical potential and activity of all phase constituents is not well defined and you cannot properly define the activity coefficients of the species in the phase.

For an aqueous solution phase, no matter what model is used, the reference state and standard state for both the solvent and solutes are defined in a special way in the Thermo-Calc software. The reference state for the solvent is set as pure water, the same as its standard state (according to Raoults's Law). The standard state for a solute species is set the hypothetical solute species, whilst its reference state is defined as the hypothetical state at unit molality (one mole dissolved into 1.0 kg of solvent) but in which the environment of each molecular is the same as at infinite dilution (according to Henry's Law). Under these definitions, the activity coefficients for solvent species can be calculated as follows:

```
RC<H2O> = ACR(H2O,aqueous)/ Y(aqueous,H2O)
```

The coefficients for the solute species can be calculated as follows:

```
RC<spec> = AI(species,aqueous)/ML(aqueous,species)
= ACR(species,aqueous)/ Y(aqueous,species)*Y(aqueous,H2O)
```

AI is here the activity of solute species calculated from the model, and ML is the molality of the species.

Thermodynamic Variables and Wildcard Characters

The ACR (species,phase) and the MUR (species,phase) quantities can only be appropriately and meaningfully applied to substitutional solution phases (such as GAS, AQUEOUS, LIQUID) and to solution phases without an interstitial sublattice set. This means that the wild card characters `*` and `$` normally don't work properly for the activity and/or chemical potential properties.

For example, do not use ACR(*,*) or MUR(*,*) for all the species relative to all phases, nor ACR(*,phase) or MUR(*,phase) for all the species relative to a specific phase, nor ACR(species,*) or MUR(species,*) for a specific species relative to all phases.

Instead, use specific names for species and (applicable) phase, as in the following examples:

```
show_value acr(fe+2,aqueous)Lists activity of the Fe+2 species in AQUEOUS solution
phase
```

```
show_value mur(c2,gas)Lists chemical potential of the C2 species in GAS mixture phase
```

```
set_axis_var y ac(o2,gas)Sets activity of the O2 species in GAS mixture phase as Y-
axis
```

Units of State Variables and Derived Variables

The units for the state variables in the Units column in the table in *User-Specified Units* below are the SI units that are used in the POLY module. However, in the POST module, you can both use pre-defined symbols and define your own symbols which are based on state variables and derived variables. By doing this, you can express the value of the thermodynamic variables in non-default units. The following topic briefly describes how you can create your own symbols and suggests expressions that you can use to convert default units into other standard units which are not default units in Thermo-Calc.

The topic *Examples of User-Defined Units* on the next page describes some variables of specific species in a phase and the units in which they are expressed. These variables are not used in POLY or POST, but in the GIBBS, DATA, PARROT and ED_EXP modules.

User-Specified Units

You do not always need to use the default units for variables. Using *ENTER_SYMBOL* on page 195, you can convert the value of variable from the default unit to your preferred unit. (Some response-driven modules also allow you to set conditions in non-default units.) User-defined symbols in the form of functions can be used for plotting in the POST module, but they cannot be used as conditions in POLY. User defined symbols in the form of variables can be used as conditions.

For example, if you want pressure to be plotted in bar rather than Pa, then you define the following function `PB`:

```
ENTER_SYMBOL FUNCTION PB = P/1E5 ;
```

If you wanted heat capacity of a system to be shown as in terms of J/mol/K, then you can define the following function Cp:

```
ENTER_SYMBOL FUNCTION CP = HM.T ;
```

If the variable you want to convert is a function of one or more derivatives, then you must enter the symbol as a variable rather as a function. For instance, a symbol expressing heat capacity of a system in a unit of cal/mol/K can be defined as the following variable `Cp2`:

```
ENTER_SYMBOL VARIABLE CP2 = HM.T/4.1858 ;
```

Also see *Examples of User-Defined Units* below for information about entering conventional functions and the associated units.

Examples of User-Defined Units

The following tables give examples of expressions you can use to enter symbols. This enables you to show the values of thermodynamic variables in a variety of units.

Units of State Variables and Derived Variables on the previous page and *User-Specified Units* on the previous page

You can also use thermodynamic variables with normalizing suffixes in the expression when you enter a symbol. However, the tables do not have examples of these expressions.

In the expressions these are defined as follows:

- `i` is for an auxiliary index or letter that corresponds to the component `c`
- `j` is for an auxiliary index or letter that corresponds to the phase `ph`, and
- `ij` stands for an auxiliary index or letter that corresponds to the component `c` in the phase `ph`.

Intensive and Extensive Variables of a Defined System

Quantity	**Suggested name and expression**	**Unit**
For intensive variables of a defined system		
Temperature	TempC = T-273.15	Celsius (C)
	TempF = 1.8*T-459.67	Fahrenheit (F)
	TempF = 1.8*TempC+32	
Pressure	PB = P/1E5	bars (bar)
	PKb = P/1E8	kilobars (kbar)
	PAtm = P/101325	atmosphere (atm)
	PSI = P/6894.76	pounds/sq. inch (psi)
	PIHg = P/3342.11	inches of Hg
	PTor = P/133.322	Tors (millimeters of Hg)

Quantity	Suggested name and expression	Unit
For extensive variables of a defined system		
Amount	BKg = 1E-3*B	kilograms (kg)
	BTon = 1E-6*B	tons
Volume	VDM = 1E-3*V	cubic decimeters (dm^3, l)
	VCM = 1E-6*V	cubic centimeters (cm^3)
	VMM = 1E-9*V	cubic millimeters (mm^3)
	VCI = 1.6387064E-5*V	cubic inches (in^3)
	VLi = 1E-3*V	liters (l)
Energy	GCal = G/4.1858	cal
	ACal = A/4.1858	cal
	UCal = U/4.1858	cal
	HCal = H/4.1858	cal
	SCal = S/4.1858	Cal/K
Heat Capacity	Cp2 = HM.T/4.1858	cal/mol/K
	Cp3 = HW.T/4.1858	cal/g/K
	Cp4 = HV.T/4.1858	cal/m^3/K
Thermal Expansion	A2 = VM.T*1E-6*VM	cm^3/mol/K
	A3 = VW.T*1E-6*VM	cm^3/g/K
Isothermal Compressibility	B2 = -VM.P*1E-9*VM	mm^3/mol/Pa
	B3 = -VW.P*1E-9*VM	mm^3/g/Pa

Intensive and Extensive Variables of a System Component

Quantity	Suggested name and expression	Unit
For intensive variables of a system component		
Chemical Potential	MUi = MU(c)/4.1858	cal/mol
	MURi = MUR(c)/4.1858	cal/mol

Quantity	Suggested name and expression	Unit
Special quantity for aqueous solution	pH = -LOG10(ACR(H+1))	dimensionless
	Eh = MUR(ZE)/RNF where RNF=96485.309	volts (V)
For extensive variables of a system component		
Amount	MFi = N(c)/N = X(c)	dimensionless
	MPi = N(c)/N*100	dimensionless
	WFi = B(c)/B = W(c)	dimensionless
	WPi = B(c)/B*100	dimensionless
	BKgi = 1E-3*B(c)	kilograms (kg)
	BToni = 1E-6*B(c)	tons

Extensive Variables of a Phase

Quantity	Suggested name and expression	Unit
Amount	MFj = NP(ph)/N	dimensionless
	MPj = NP(ph)/N*100	dimensionless
	WFj = BP(ph)/B	dimensionless
	WPj = BP(ph)/B*100	dimensionless
	BKgj = 1E-3*BP(ph)	kilograms (kg)
	BTonj = 1E-6*BP(ph)	tons
Volume	VCMj = 1E-3*V(ph)	cubic decimeters (dm^3, l)
	VCMj = 1E-6*V(ph)	cubic centimeters (cm^3)
	VMMj = 1E-9*V(ph)	cubic millimeters (mm^3)
Energy	GCalj = G(ph)/4.1858	cal
	ACalj = A(ph)/4.1858	cal
	UCalj = U(ph)/4.1858	cal
	HCalj = H(ph)/4.1858	cal
	SCalj = S(ph)/4.1858	Cal/K

Quantity	Suggested name and expression	Unit
Driving Force	DG2j = DGM(ph)/4.1858	cal/mol
	DG3j = DGW(ph)/4.1858	cal/g
	DG4j = DGV(ph)/4.1858	Cal/m^3
	DG5j = DGF(ph)/4.1858	cal/mole_formula_unit
Heat Capacity	Cp2j = HM(ph).T/4.1858	cal/mol/K
	Cp3j = HW(ph).T/4.1858	cal/g/K
	Cp4j = HV(ph)/.T/4.1858	cal/m^3/K
	Cp5j = HF(ph)/.T/4.1858	cal/mole_formula_unit/K
Thermal Expansion	A2j = VM(ph).T*1E-6*VM	cm^3/mol/K
	A3j = VW(ph).T*1E-6*VM	cm^3/g/K
	A4j = VF(ph).T*1E-6*VM	cm^3/mole_formula_unit/K
Isothermal Compressibility	B2j = -VM(ph).P*1E-9*VM	mm^3/mol/Pa
	B3j = -VW(ph).P*1E-9*VM	mm^3/g/Pa
	B4j = -VF(ph).P*1E-9*VM	mm^3/mole_formula_unit/Pa

Extensive Variables of a Component in a Phase

Quantity	Suggested name and expression	Unit
Amount	MFij = N(ph,c)/NP(ph) = X(ph,c)	dimensionless
	MPij = N(ph,c)/NP(ph)*100	dimensionless
	WFi = B(ph,c)/BP(ph) = W(ph,c)	dimensionless
	WPij = B(ph,c)/BP(ph)*100	dimensionless
	BKgij = 1E-3*B(ph,c)	kilograms (kg)
	BTonij = 1E-6*B(ph,c)	tons

Intensive and Extensive Variables of a Species in a Phase

Quantity	**Suggested name and expression**	**Unit**
For intensive variables of a species in a phase		
Chemical Potential	MUCalij = MU(sp,ph)/4.1858	cal/mol
	MUErgij = MU(sp,ph)*1E7	cal/mol
Fugacity	FAij = AC(sp,ph)*PATM	atmosphere (atm)
	FBij = AC(sp,ph)*PB	bars (bar)
	FCij = AC(sp,ph)*PKB	kilobars (kbar)
	FTij = AC(sp,ph)*PTOR	Tors (millimeters of Hg)
ln(Fugacity)	LnFAij = LNAC(sp,ph)+LN(PATM)	atmosphere (atm)
	LnFBij = LNAC(sp,ph)+LN(PB)	bars (bar)
	LnFCij = LNAC(sp,ph)+LN(PKB)	kilobars (kbar)
	LnFTij = LNAC(sp,ph)+LN(PTOR)	Tors (millimeters of Hg)
Special quantity for aqueous solution	AIij=ACR(FE+3,AQ)*AH2O	dimensionless
	RCij=ACR(FE+3,AQ)*YH2O/Y(AQ,FE+3) where AH2O=55.508435 and YH2O=Y(AQ,H2O)	dimensionless
	WRCalij = WR(AQ,sp)/4.1858 (WR(AQ,sp) is only valid for aqueous species in a system in which the AQUEOUS solution phase is considered)	cal/mol
For extensive variables of a species in a phase		
Special quantity for aqueous solution	MLij=Y(AQ,FE+3)*AH2O/YH2O	molality (m)
	ISTR=1*IS1+1*IS2+1*IS3 where AH2O=55.508435, YH2O=Y(AQ,H2O) and ISn=.5*MLi*Zi**2+.5*MLj*Zj**2+.5*MLk*Zk**2	molality (m)

Units for Variables of Specific Species in a Phase

In the GIBBS, DATA, PARROT and ED_EXP modules, there are quantities that describe various thermodynamic, physical, chemical and transport properties for a compound phase, and for a certain species or a given species combination in a specific solution phase. The following table describes the units for those variables.

These variables cannot be directly used in the POLY or POST modules.

Variables	Description and unit
G(ph,sp) G(ph,sp;0) G(ph,sp1;sp2;...;0)	Gibbs energy (J/mol) of a pure substance or end-member.
G(ph,sp1,sp2,...) L(ph,sp1,sp2,...) G(ph,sp1,sp2,...;0) L(ph,sp1,sp2,...;0) G(ph,sp1,sp2,...;...;0) L(ph,sp1,sp2,...;...;0)	Zero-order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
G(ph,sp1,sp2,...;i) L(ph,sp1,sp2,...;i) G(ph,sp1,sp2,...;...;i) L(ph,sp1,sp2,...;...;i)	The ith -order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp) TC(ph,sp;0) TC(ph,sp1;sp2;...;0)	Curie temperature (K) of a pure substance or end-member.
TC(ph,sp1,sp2,...) TC(ph,sp1,sp2,...;0) TC(ph,sp1,sp2,...;...;0)	Zero-order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp1,sp2,...;i) TC(ph,sp1,sp2,...;...;i)	The ith -order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.

Variables	Description and unit
BMAGN(ph,sp) BMAGN(ph,sp;0) BMAGN (ph,sp1;sp2;...;0)	Bohr magneton number (dimensionless) of a pure substance or end-member.
BMAGN (ph,sp1,sp2,...) BMAGN (ph,sp1,sp2,...;0) BMAGN (ph,...;sp1,sp2,...;0)	Zero-order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
BMAGN (ph,sp1,sp2,...;i) BMAGN (ph,sp1,sp2,...;...;i)	The ith -order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp) V0(ph,sp;0) V0(ph,sp1;sp2;...;0)	Molar volume (m^3) at 1 bar and reference T0 of a pure substance or end-member.
V0(ph,sp1,sp2,...) V0(ph,sp1,sp2,...;0) V0 (ph,sp1,sp2,...;...;0)	Zero-order composition-dependent molar volume (m^3) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp1,sp2,...;i) V0 (ph,sp1,sp2,...;...;i)	The ith-order composition-dependent molar volume (m^3) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VA(ph,sp) VA(ph,sp;0) VA(ph,sp1;sp2;...;0)	Integrated thermal expansivity (m^3/mol/K) of a pure substance or end-member.
VA(ph,sp1,sp2,...) VA(ph,sp1,sp2,...;0) VA (ph,sp1,sp2,...;...;0)	Zero-order composition-dependent thermal expansivity (m^3/mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.

Variables	Description and unit
VA(ph,sp1,sp2,...;i) VA (ph,sp1,sp2,...;...;i)	The ith -order composition-dependent thermal expansivity (m^3/mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp) VB(ph,sp;0) VB(ph,sp1;sp2;...;0)	Isothermal compressibility (m^3/mol/Pa) of a pure substance or end-member.
VC(ph,sp1,sp2,...) VB(ph,sp1,sp2,...;0) VB (ph,sp1,sp2,...;...;0)	Zero-order composition-dependent isothermal compressibility (m^3/mol/Pa) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp1,sp2,...;i) VB (ph,sp1,sp2,...;...;i)	The ith -order composition-dependent isothermal compressibility (m^3/mol/Pa) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VK(ph,sp) VB(ph,sp;0) VB(ph,sp1;sp2;...;0)	High-pressure fitting parameter (m^3/mol) of a pure substance or end-member.
VK(ph,sp1,sp2,...) VB(ph,sp1,sp2,...;0) VB (ph,sp1,sp2,...;...;0)	Zero-order composition-dependent high-pressure fitting parameter (m^3/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VK(ph,sp1,sp2,...;i) VB (ph,sp1,sp2,...;...;i)	The ith -order composition-dependent high-pressure fitting parameter (m^3/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
WR(ph,sp) WR(ph,sp;0)	Standard Born function (J/mol) of a specific aqueous species in the AQUEOUS solution phase (always with a single sublattice) under the reference-state temperature and pressure.

Data Optimization User Guide

Thermo-Calc Version 2016b

Introduction

In this section:

Introduction to Data Optimization

This user guide describes the basic idea behind data optimization, contains brief descriptions of the modules and file types that you work with while doing your optimization, as well as rough outline of overarching workflow that you typically follow when working with optimization.

This guide assumes that you are familiar with using the Thermo-Calc Console Mode. It also assumes that you understand the principles of thermodynamics and are familiar with the theoretical foundations of computational thermodynamics.

Also see the *Thermo-Calc Console Mode Command Reference* included with this documentation set, which has information about all the commands available in the Thermo-Calc Console Mode, including PARROT and ED_EXP. Note that the commands listed under PARROT and ED_EXP are only commands that are specific to PARROT and/or ED_EXP. These modules also contain some commands that are also available in POLY.

Example 36 in the *Console Mode Examples Guide*. It is a detailed example of assessment and optimization in Thermo-Calc.

Data Optimization

In a thermodynamic database, each phase in a system is characterised using a mathematical model of its Gibbs energy. The Gibbs energy of a phase depends on various state variables. It can be defined individually even in a heterogeneous system with many stable phases since the properties of one phase are completely independent of the properties of the other phases in the system. In most alloy systems, the thermodynamic properties of a phase can be modelled by expressing how the Gibbs energy depends on temperature and composition. State variables such as pressure, volume or entropy can also serve as parameters in the Gibbs energy expression. The Gibbs energy of the whole system is the sum of the products of the Gibbs energy of each phase multiplied by the amount of that phase.

How the Gibbs energy of the phase varies with various state variables is determined by a mathematical model and how various adjustable parameters of the model is set. By optimizing these parameters, you can calculate the thermodynamic properties of a system under various conditions (by calculating phase diagrams for example). The thermodynamic properties themselves are functions of temperature, pressure or composition. They include, among other properties, standard enthalpy of formation, entropy, heat capacity, molar volume, thermal expansivity, compressibility and Curie temperature for magnetic transformations.

Data optimization is about adjusting the model parameters so that calculated equilibria fit well with experimental data. An important part of a data optimization is therefore collecting and assessing available experimental and theoretical information about phase equilibria and thermochemical properties of a system.

When you optimize the parameters of the model of a phase, you put what is called optimizing variables into the Gibbs energy expressions of those parameters. During the optimization, the values of these variables are varied in order to find a fit between the calculated equilibria and the experimental data that you base the optimization on. Once you have settled on a Gibbs energy expression for a certain parameter of a phase of the element, then you must stick to this expression in all future optimizations involving the element. If you do not do this, then you must re-optimize all previous systems that involve this element when the expression is changed.

The Thermo-Calc software allows you to optimize parameters that characterize not only binary systems, but also ternary system and systems of even higher orders. You can even optimize parameters that characterise systems of different orders at the same time.

The Least-Squares Method

Data optimization in Thermo-Calc is based on the least-squares method for fitting values calculated on the basis of a model with observed quantities. The software is accordingly trying to find the optimizing variable values that lead the minimized sum of the squares of the differences between the calculated values and the observed quantities (that is, of the errors or residuals).

The least-squares method works best under the following conditions:

- The observed quantities have a Gaussian probability distribution.
- The observed quantities are only subject to random errors.
- The different observations (experiments) are uncorrelated
- The standard deviation of each observation can be estimated.
- The number of observations is large.
- The models used give precise predictions.

Of course, these conditions are usually not all met in a normal thermodynamic assessment. But even in non-ideal conditions, there is no known method that works better than the least-squares method.

The CALPHAD Approach

The data optimization functionality in Thermo-Calc works according to the CALPHAD approach to computational thermodynamics. This approach builds on the development of models that accurately represent thermodynamic properties for various phases. These models enable you to predict the thermodynamic properties of multicomponent systems-based data concerning binary and ternary subsystems. The predictions can take many factors into accounts, such as, for example, crystallography, type of bonding, order-disorder transitions and magnetic properties.

CALPHAD is originally an abbreviation of *CALculation of PHAse Diagrams*, but as the approach has expanded in scope, it now stands for *computer coupling of phase diagrams and thermochemistry*.

References

For in-depth information about CALPHAD as well as data optimization, see *Computational*

Thermodynamics – The Calphad Method by Hans Leo Lukas, Suzana G. Fries and Bo Sundman (Cambridge University Press, 2007). CALPHAD was given its first general description in *Computer Calculations of Phase Diagrams* by Larry Kaufman and Harold Bernstein (Academic Press, 1970). The book contains some case studies of optimizations using Thermo-Calc.

Information about the concept of 'lattice stability' (which is important for the development of multicomponent thermodynamic databases) can also be found in the paper *Hume-Rothery and Calphad Thermodynamics* by Larry Kaufman, published in *Calphad and Alloy Thermodynamics*, edited by Patrice E.A. Turchi, Antonios Gonis, Robert Shull (The Minerals, Metals & Materials Society, 2002), pp. 3-19.

Working with Data Optimization in Thermo-Calc

In this section:

Data Optimization in Thermo-Calc

The actual performance of the optimization of a system is primarily done in the PARROT module, and in its sub-module ED_EXP. The POLY and POST modules are used to calculate and plot property or phase diagrams based on the optimized variables. This allows you to visually assess how good a fit you have achieved between your calculated results and your experimental data.

The end result of a successful optimization is typically an updated Thermo-Calc database file (with filename extension *.TDB) or a new database file.

Data Optimization Workflow

When you carry out an optimization using Thermo-Calc, you typically follow a workflow as outlined below.

1. Collect experimental data about your system from various sources such as journal articles and reports.
2. Create a POP-file in which you enter the experimental data you have collected.
3. Create a setup macro file in which you define your system and the variables you want to optimize. A useful general procedure is to first find a minimum set of variables that allows you to calculate most of the experiments.
4. Run the setup macro file.
5. Compile your POP-file. This file often contains errors, which need to be corrected, and the file recompiled several times before the compilation is completed without errors.
6. In the ED_EXP module, check that the experiments in your POP-file reach equilibrium with reasonable results. If any experiments do not reach equilibrium with reasonable results, then try changing the starting values on equilibrium conditions (such as composition) to see whether the equilibrium can be computed after all. If this does not work, then you can temporarily exclude the experiment from the optimization. At a later stage in the optimization, when the optimizing variables have different values, you can check whether the experiments can be computed with reasonable results.
7. Back in the PARROT module, run the first optimization cycle and evaluate the feedback in the console. You can also plot diagrams in the POLY module that allow you to visually inspect the fit between calculated optimization results and the experimental data. If you are not satisfied with the fit, then enter the ED_EXP module again and adjust the weights of the experiments in a way that is likely to improve the fit and run another optimization cycle. Reiterate until you are satisfied with the fit.
8. Once you get the optimization stable and smooth with the minimum set of variables chosen in step 3 above, try using different sets of variables to see whether improvements are possible.

9. When you are satisfied with the fit between calculated results and experimental data with your final set of optimizing variables, update your setup file and POP-file. In the setup file, enter the calculated optimizing variable values as the variables' start values. In the POP-file, enter the final weights of the experiments. With these files updated, you can easily regenerate the parameter values of your optimized system. Having the files updated also makes it easier to optimize the system again in light of new data or new theoretical models.
10. Finally, update the database with your calculated results or create a new database with information about the system that you have optimized.

The PARROT Module

The PARROT module consists of a comprehensive subroutine package for data evaluation of thermodynamic model parameters from experimental data. The module has 99 variables that you can use for optimization and the module can handle a thousand experimental measurements in an optimization. However, there are limits on the simultaneous numbers of variables and experiments. These limits are listed at each optimization.

The PARROT module is part of the Thermo-Calc software. The module is not included in the software development kits TQ-Interface, TC-API or TC-Toolbox for MATLAB®.

The experimental data is entered and edited in a sub-module of PARROT: *The EDIT_EXPERIMENTS Module* below.

The EDIT_EXPERIMENTS Module

The EDIT_EXPERIMENTS module, or ED_EXP for short, is used for entering, evaluating and editing experimental data. To enter the module, go to *The PARROT Module* above and then issue the command *EDIT_EXPERIMENTS* on page 95.

Since ED_EXP uses the POLY module for doing equilibrium calculations of experimental data points, many POLY commands are also available in the ED_EXP module. However, the commands may work somewhat differently in the two modules. There are also unique ED_EXP commands which are not found in POLY.

When you execute ED_EXP commands, the PARROT workspace is modified. However, note that you must always first use *READ_WORKSPACES* on page 160 in ED_EXP before doing anything in the module. The command loads the experimental data that you are going to work with during the optimization. Furthermore, before leaving ED_EXP you must use *SAVE_WORKSPACES* on page 30 or the results of your work in the ED_EXP module is lost.

Data Optimization in Other Modules

All kinds of thermodynamic data, calculated equilibrium states or dynamic parameters are transferred back and forth between the PARROT and the GIBBS module as well between these and the POLY module. Whenever an optimization run is performed, PARROT calls the GIBBS module for stored system definition data and model parameters.

In Thermo-Calc, the GIBBS module (the Gibbs Energy System) handles the models of the various phases that can form in a multicomponent system. It stores thermodynamic data and performs various Gibbs energy equilibrium calculations. It contains subroutines to analytically calculate the first and second partial derivatives of integral Gibbs energy with respect to any set of variables. Many thermodynamic models for various types of substances are implemented in the module. Some commands that are available in the PARROT module are also available in the GIBBS module.

In the GIBBS module, parameters of the Gibbs energy models are referred to as *TP-functions*.

PARROT calls the POLY module for equilibrium calculations. The POLY module is used for calculating and storing complex heterogeneous equilibria.

Optimization File Types

These are the important files you work with when optimizing.

File type	**Description**
POP-file	The POP-file (Parrot OPtimization file) is the file that contains all the experimental data that you use for optimizing Gibbs energy values for your system. The POP-file is a plain text file that contains ED_EXP commands. By default, the file has the filename extension *.POP in Thermo-Calc.
Setup file	The setup file is a Thermo-Calc macro file (*.TCM). This file typically contains commands that define your system, opens the PARROT workspace (and associated GIBBS and POLY workspaces) and sets optimizing variables.
Other macro files	It is often useful to have other macro files than the setup file at hand while you are doing your optimization. For example, it is convenient to have a macro file that automatically plots phase diagrams or other diagrams based on the latest values of your optimizing variables. An optimization process typically involves many optimization cycles, so this operation needs to be done many times during a typical optimization.
Workspace files	The PARROT module has its own workspace with dynamic memories, similar to the workspaces of POLY and GIBBS. It is stored and updated in a PARROT workspace file with the filename extension *.PAR. The workspace file is a binary file whose format is hardware dependent. This means that the format is unique for each type of CPU. Hence, a workspace file saved on a computer with one type of CPU cannot be used on a computer with another type of CPU.

File type	Description
EXP-file	The EXP-file is a plain text file with information in the form of DATAPLOT Graphical Language commands. These commands can specify some or all of the data points in your POP-file. This allows you to plot these data points on top of your plotted optimization results (with the POST commands *APPEND_EXPERIMENTAL_DATA* on page 192 or *QUICK_EXPERIMENTAL_PLOT* on page 201). You can then visually assess the fit between these results and the experimental data. The PARROT workspace is not influenced in any way by the creation or use of EXP-files. Also see the *DATPLOT User Guide* included with this documentation set.

Optimization Workspaces

When writing the setup file, you enter a *CREATE_NEW_STORE_FILE* on page 94 command which creates a PARROT workspace file. Alternatively, select an existing PARROT workspace file with *SET_STORE_FILE* on page 116. The workspace file is automatically updated and saved with the latest optimization results (after each use of the *OPTIMIZE_VARIABLES* on page 109 command). You can also explicitly instruct Thermo-Calc to save the workspace using *SAVE_PARROT_WORKSPACES* on page 111. If you want to get rid of your latest changes and return to the state of your workspace when it was last saved, use *READ_PARROT_WORKSPACES* on page 109.

When the PARROT workspace is saved, parts of the POLY and GIBBS workspaces are also saved to the PARROT workspace file, along with the PARROT workspace itself. Using the POLY command *SAVE_WORKSPACES* on page 161 creates a new POLY3 file, nothing is saved to the PARROT workspace file.

If you do any POLY calculations based on data in the current workspace file, then a *.POLY3 file is created, which contains a copy of the current set of parameters. If you continue on your optimization and read the old *.POLY3 file, then the new set of parameters is overwritten with the old set. It is therefore recommended that you never read a *.POLY3 or *.GES5 file while you are doing an optimization.

Method for Optimization and Simulation

The PARROT module typically uses ordinary POLY minimization for equilibrium calculations. The global minimization technique that is used in POLY cannot be used because it automatically creates new composition sets which corrupt the PARROT workspace. Furthermore, the equilibrium definitions that you use as input for your optimization must each be attributed to a specific phase. Some of these definitions may specify some local or partial equilibrium state rather than a global minimum. However, it is possible to use the global minimization technique for some equilibrium calculations by using the ED_EXP command *ADVANCED_OPTIONS* on page 125 with the `Toggle_Alternate` option.

Optimization in PARROT is performed on the basis of a ‘maximum likelihood’ principle. According to this principle, the best fit between various calculated results and all the input of experimental data is found where the sum of the square of the weighted residuals is at its minimum.

Typically, the results of an optimization is considered to be better the fewer optimizing variables that are needed to get the same level of fit between computed results and experimental data. If you can get almost the same fit using eight instead of twelve parameters, then this should be considered to be a significant improvement. When more parameters are used, the values of the individual parameters tend to become unrealistic. This is particularly true when it comes to temperature-dependent parameters. However, relatively small differences in the number of parameters are often insignificant. For example, it does not typically matter whether you used 24 or 25 parameters to reach a certain degree of fit.

It is often difficult to compare the quality of different optimizations based on the number of optimizing variables that have been optimized. Since you may rely more or less heavily on different pieces of available experimental data (and do so with good reason), it is possible that two different users could end up with very different numbers of parameters for the same system. For example, suppose you optimize the Fe-Al system to incorporate it into an Al database, while someone else optimizes the same system to incorporate it into an Fe database. In this situation, the two of you would probably make different judgements about which experimental information your calculated results must have a good fit with.

Creating the POP-File

Before starting an optimization in Thermo-Calc, you must collect relevant experimental data about your system that is available in the research literature. This data is then entered in the POP-file. The experimental data points and measurements are entered in this plain text file in the form of ED_EXP commands.

The syntax of the POP-file is in principle independent of the models used for describing the phases in the system.

In this section:

Experimental Information

An optimization of thermodynamic model parameters should be based on a range of reliable experimental results that is as wide as possible, as well as on empirical or semi-empirical correlations and theoretical considerations. During an optimization in Thermo-Calc, many kinds of thermochemical and thermophysical data can be mixed and used together.

The information needed for an optimization represent measurements of thermodynamic parameters in the system at equilibrium. These can be measurements of any of the thermodynamic quantities that can be set as conditions in Thermo-Calc. The information may represent measurements of activities or enthalpies in single-phase regions for example, or solubilities or transformation temperatures in a multi-phase region.

For each equilibrium that is used in the optimization, at least one quantity must have been measured and you also need to know the conditions that must be set to compute the system's equilibrium state. For example, consider a binary system in a single-phase region. Suppose that you have measured the temperature, pressure, composition and the chemical potential. Three of these quantities are necessary to specify the equilibrium state and the forth can be used as experimental information to model the phase.

If you have a two-phase region and know the temperature and pressure conditions, as well as which the stable phases are, then you could use the compositions of one or both phases as experimental data. The former information about the conditions is sufficient to determine the equilibrium. The experimental information can then be used to optimize the parameters that are used to characterise and model the system.

For examples how to enter various kinds of experimental data in the POP-file, see *Experiments and Experimental Data* on page 50.

Conflicting or Missing Information

You are likely to sometimes have inconsistent or conflicting experimental information. In principle, all available experimental data should still be entered into the POP-file, unless you have good reasons to exclude some information. For example, if you have reason to believe that the samples used in some experiments were not pure, then these experiments could be excluded from the POP-file.

For some systems, you have very little experimental data to go on. When this is the case, do not try to fit the available data uncritically with high accuracy without considering possible errors. You can look for data in systems with similar elements to get an idea about what the reasonable estimates of data that is lacking could be. Or you can use calculations from first principles or semi-empirical methods to get reasonable estimates that can be used as experimental data.

Invariant Equilibria Information

The most valuable experimental information for an optimization is information about stable invariant equilibria. An invariant equilibrium is such that neither pressure, temperature nor composition can be changed without there being a change in the set of phases present in the system. It is recommended that all information about invariant equilibria for a system is included in the POP-file. These equilibria need not all be based on explicit experimental measurements of thermodynamic properties.

Reasonable estimates from available experimental data are often useful to include in the POP-file. Such estimates, which should be based on the available experimental data, helps Thermo-Calc find a good set of start values on the optimization variables. However, at the end of the assessment, these estimated equilibria should be excluded and you should complete the optimization based only on the experimental information that is based on measurements.

With some experience from phase diagram evaluation, it is possible to make reasonable estimates of metastable invariant equilibria. Such estimates helps reduce the number of phases that are assessed simultaneously during the optimization. For example, you may assume that a certain intermediate phase does not form in a system. Then extrapolate the liquidus curves below the stable three-phase equilibria and finally, estimate temperatures and compositions of metastable three-phase equilibria between two other phases and the liquid.

Another useful technique is to extrapolate a liquidus line from a peritectic equilibrium to estimate the congruent melting temperature of a compound. This estimate may be more useful than the information about the peritectic equilibrium itself as the equilibrium involves only two phases.

Equilibria in Higher-Order Systems Information

When you optimize a binary system, the available experimental information can often be described equally well by very different sets of parameters. Information about ternary and higher order systems that include the components of the binary system are then often useful for optimizing the binary system (the same is true of information about quaternary system with respect to optimizing ternary systems). Often, it is only when you extrapolate the optimized parameters to a higher-order system that you can judge which of the sets of model parameters that is best. Sometimes information from several ternary systems is required to make a reliable judgement about which set of parameters best describes a particular binary system.

Heat Capacities Information

If you want to optimize your system based on data about heat capacities, then the corresponding parameters should first be optimized separately before you perform the general optimization of your system. The parameters should be kept fixed during the general optimization. This is because it is normally not possible to optimize heat capacity data together with other data in a meaningful way. If you do this, then it is very likely that the parameters related to the heat capacity are badly determined.

POP-File Syntax

It is recommended that you specify an experimental equilibrium as close as possible to actual experimental conditions. Ideally, there is information about the set of stable phases, temperature, pressure and some or all compositions for the equilibrium.

In addition, it is recommended that you keep the POP-file well-organised and extensively commented. This is especially important if someone else reassesses the system when new experimental information is available.

If you have too many equilibria defined in your file, or if you define equilibria with different sets of components in the same file, then you must divide the POP-file in *blocks* (using the *FLUSH_BUFFER* on page 41 command). You know whether you have defined too many equilibria for one block when you compile the file. A too large number of equilibria leads to an error message when the file is compiled.

If you use the *DEFINE_COMPONENTS* on page 143 command, then it must be the first command in the POP-file (or if you have several blocks, DEFINE_COMPONENTS can also be put as the first command after FLUSH_BUFFER). This is because the command automatically reinitiates the current workspace, so the effect of any commands placed before it are not saved.

The last command in the POP-file should always be *SAVE_WORKSPACES* on page 30.

Legal Commands in a POP-File

The following commands can be used in a POP-file.

Also see the *Thermo-Calc Console Mode Command Reference Guide*for information about all these commands.

- *ADVANCED_OPTIONS* on page 125
- *CHANGE_STATUS* on page 135
- *COMMENT* on page 40
- *CREATE_NEW_EQUILIBRIUM* on page 143
- *DEFINE_COMPONENTS* on page 143
- *ENTER_SYMBOL* on page 195
- *EVALUATE_FUNCTIONS* on page 155
- *EXPERIMENT* on page 24
- *EXPORT* on page 26
- *FLUSH_BUFFER* on page 41
- *IMPORT* on page 27
- *LABEL_DATA* on page 28
- *SAVE_WORKSPACE* on page 232
- *SET_ALL_START_VALUES* on page 162
- *SET_ALTERNATE_CONDITION* on page 30
- *SET_CONDITION* on page 165
- *SET_NUMERICAL_LIMITS* on page 237

- *SET_REFERENCE_STATE* on page 169
- *SET_START_VALUE* on page 171
- *SET_WEIGHT* on page 33
- *TABLE_HEAD, TABLE_VALUES and TABLE_END* on page 39

Entering Experimental Information

A POP-file in Thermo-Calc (*.POP) mainly consists of descriptions of equilibria, each equilibrium describing a data point that is based on an experiment from the existing literature on your system. An equilibrium is specified using ED_EXP commands.

The following is an example of a specification of an equilibrium with a single stable phase in the Au-Cu system. Equilibria with a single stable phase are often from experiments where enthalpies of mixing or chemical potentials have been measured.

```
CREATE_NEW_EQUILIBRIUM 1 1

CHANGE_STATUS PHASE LIQUID=FIX 1

SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563

SET_REFERENCE_STATE AU LIQ * 1E5

SET_REFERENCE_STATE CU LIQ * 1E5

EXPERIMENT HMR=-1520:200

COMMENT Measurement by Topor and Kleppa, Met trans 1984
```

Creating a New Equilibrium

The first command in an equilibrium specification is always *CREATE_NEW_EQUILIBRIUM* on page 143. This command takes two integers as arguments. The first integer should specify a unique identifier that can be used later to refer to the equilibrium in question. The second integer is an initialisation code 0, 1 or 2:

- Code 1: This means that all components are entered but all phases are suspended. This code is appropriate in most cases.
- Code 0: This means that all components and phases in the equilibrium are suspended initially. This code is needed if you are using experimental data about systems of different orders simultaneously, such as data about both binary and ternary systems for example.
- Code 2: This means that all components and phases are initially entered.

Example

For example, the first command in the example above creates an equilibrium data point with the unique identifier 1. All components of the system are entered but all phases are suspended:

```
CREATE_NEW_EQUILIBRIUM 1 1
```

Setting Equilibrium Conditions and its Uncertainty

All the equilibrium-related commands that are placed in between two *CREATE_NEW_EQUILIBRIUM* on page 143 commands are interpreted as specifying the conditions of the equilibrium created by the first command. The values of these conditions should be based on the conditions specified in the experiment that you base the equilibrium definition on.

Example

In the example, the *CHANGE_STATUS* on page 59 command specifies that the equilibrium is a single-phase equilibrium with the liquid phase.

```
CHANGE_STATUS PHASE LIQUID=FIX 1
```

Furthermore, the temperature is 1379 K, the pressure is 1 bar (1E5 Pa) and the mole fraction of Au is 0.0563.

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563
```

Sometimes you have reason to think that some information about an equilibrium condition may not be accurate. If this is the case, then you specify the degree of uncertainty for a condition with a colon after the condition quantity, directly followed by either an absolute value or a percentage. For example, if you have reason to doubt the reliability of the Au mole fraction measurement, then you could write:

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563:10%
```

This indicates that you think the Au mole fraction is between 0.0507 and 0.0619. PARROT calculates the equilibrium twice, once for 0.0507 and once for 0.0619, and then computes the change of each experimental value between these two equilibria. This change is used to modify the uncertainty specified for the experimental value.

Also see *Entering the Experimental Value and its Uncertainty* on the next page.

The possibility of specifying uncertainties on conditions may be useful when you have experimental data about a ternary system. In a binary system, a tie-line is determined by the two phases, the temperature and the pressure. Measurements of the compositions of both phases can then be used as experimental data. To specify the tie-line in a ternary two-phase equilibrium one of the four compositions must also be set as a condition. If the measurement of this composition has the same uncertainty as the other compositions, then you can assign this same degree of uncertainty both to the composition selected as a condition and the compositions selected as experimental data. Alternatively, the sample (overall) composition could be used as a condition and all four phase compositions could be used as experiment values. These phases must have the status *entered* (not fixed) since the relative amount of each is unknown.

Setting Reference States

If you want to specify a non-default reference state for one or several of your system components, then you do this with the *SET_REFERENCE_STATE* on page 169 command. In the following example, the reference state for the liquid phase is set to current temperature (*) and a pressure of 1E5 Pa.

Example

```
SET_REFERENCE_STATE AU LIQ * 1E5
SET_REFERENCE_STATE CU LIQ * 1E5
```

Note that in order for these reference states to be taken into account when the measurement of the enthalpy per mole of the system is entered with experiment, the R-suffix must be used.

Entering the Experimental Value and its Uncertainty

The *EXPERIMENT* on page 24 command is used to specify the quantity that the calculated results should be fitted to. When specifying this quantity, you both specify the measured quantity itself and your estimation of the uncertainty of this value.

Example

In the example, the EXPERIMENT command specifies the enthalpy per mole of the system, where this value is specified with respect to non-default reference states that you have set in the equilibrium specification:

```
EXPERIMENT HMR=-1520:200
```

The value before the colon is the quantity of the variable. The value after the colon is an assessment of the uncertainty of this quantity. A higher value means a greater uncertainty. In the example, the uncertainty has been specified with an absolute value but it could also be specified in percent of the quantity:

```
EXPERIMENT HMR=-1520:13%
```

Several experiments can be specified after the experiment command. Besides assigning values to conditions, it is also possible to specify that a certain quantity is greater than or less than a certain value. For instance, the following command would specify that the activity of the C-component is less than 0.01 and the mass fraction of the BCC phase of Ag is greater than 0.05:

```
EXPERIMENT ACR(C)<0.01:0.001 W(BCC,AG)>0.05:10%
```

Note that an experimental quantity can typically also be treated as an equilibrium condition, and vice versa. Which measured quantities that you treat as conditions and which quantities you treat as experimental data should be based on the accuracy of the different measurements. In most cases, the quantity that is based on the experimental technique with the lowest accuracy should be used as the experimental value.

Entering Many Equilibria as a Table

When one thermodynamic variable (e.g. heat capacity) has been measured as a function of another (e.g. temperature), then experimental data is often presented as a table. By using the TABLE_HEAD, TABLE_VALUES and TABLE_END commands, you can enter such experimental information into the POP-file in the form of a table. These three commands should always be used together and must be entered in the right order. See *TABLE_HEAD, TABLE_VALUES and TABLE_END* on page 39.

The TABLE_HEAD command is followed by a number. This number identifies the table as a whole, but also uniquely identifies the first equilibrium that is included in the table. This numeric identifier is incremented by one for each additional equilibrium in the table. Each row in the table represents one equilibrium. Thus, the equilibrium defined by the first row in the table above (on the line immediately below TABLE_VALUE) is uniquely identified with the number 1, the equilibrium defined by the second row by number 2, and so on until the last equilibrium on the sixth row, which is identified by the number 6.

Since the unique identifiers of the equilibria in the table are automatically generated from the unique numerical identifier that you give to the table, the unique numerical identifier that is normally given to the *CREATE_NEW_EQUILIBRIUM* on page 143 command is replaced by two at signs (@@).

At least one of the equilibria conditions specified with the *SET_CONDITION* on page 165 command must be a condition whose value is set by the numbers in one of the table columns. To assign the numbers in a column to a condition, use the syntax SET_CONDITION `<condition>=@<column number>`. For instance, in the example above, the mole fraction of X(ALO3/2) is for each equilibrium given by the number in the first column of the table.

At least one of the measured variables that are entered with the experiment command must be a variable whose value is set by the numbers in a table column. To assign the numbers in a column to a measured variable, use the syntax EXPERIMENT `<variable>=@<column number>`. In the example above, the measured temperature for each equilibrium is given by the number in the second table column.

The actual table should be entered between TABLE_VALUES and TABLE_END. Separate the columns with tabs or any number of spaces. The columns do not have to contain numbers, but can also contain other types of values, such as phase names for example. If a column contains text with spaces or special characters, then the text must be surrounded by double quotes (“`ABC DEF&ghi`”, for example). The table may have columns that are not used, but each row must have exactly the same number of columns.

Example

The following block of commands exemplifies how a table can be entered into a POP-file:

```
TABLE_HEAD 1

CREATE_NEW_EQUILIBRIUM @@ 1

CHANGE_STATUS PHASE TETR=FIX 0

CHANGE_STATUS PHASE ION=ENT 1

SET_CONDITION P=101325 N=1 ACR(O2,GAS)=.21 X(ALO3/2)=@1

EXPERIMENT T=@2:5

TABLE_VALUE

0.46082476

0.57142380

0.66822276

0.7496 2176

0.50382426

0.63132249

TABLE_END
```

Setting Site Fraction Start Values

In some systems, you have to set non-default composition start values on some experiments in order to get them to converge properly during optimization. This may be important if your system has a miscibility gap for example, in which case several equilibria with different compositions exist at certain temperatures. In such cases, you have to make sure it is specified in the POP-file which side of the miscibility gap the equilibrium is on. The calculated equilibrium could otherwise end up on the wrong side, resulting in a large error.

In the POP-file, you can set the site fraction of a constituent on an equilibrium with *SET_START_VALUE* on page 171.

Example

For example, the following command sets the composition start value of VA constituent of the FCC_A1 phase to 0.99:

```
SET_START_VALUE Y(FCC_A1,VA#2)=0.99
```

Setting the mole fraction for a component in a phase is not as reliable as setting the site fraction.

Additional equilibria entered after the last SET_START_VALUE command are automatically given a similar start value if the following command appears previously in the POP-file:

```
SET_ALL_START_VALUES Y
```

If start values are not set automatically for phase constituents, then you may have to set the composition start value for each equilibrium (or table of equilibria) separately.

Commenting About an Equilibrium

The COMMENT command inserts a comment about the equilibrium that is saved to the PARROT workspace file when the POP-file is compiled. The comment must be entered on one line.

Comments can also be entered immediately after a dollar sign ($), but these are not saved to the PARROT workspace. Instead, these comments are ignored by Thermo-Calc when the POP-file is compiled.

Simultaneous Use of Binary and Ternary Experiments

You can use experimental information about binary and ternary systems (as well as systems of even higher order) in the same POP-file and optimization. To do this, you must inform the PARROT module that not all components of the ternary system (or system of even higher order) should be considered. This allows you, for example, to use experimental information about a binary equilibrium that exists within a ternary system.

Use *CHANGE_STATUS* on page 59 with the keyword component and which components that should be entered. You should also give the initialization code 0 (rather than 1) to the *CREATE_NEW_EQUILIBRIUM* on page 143 command. This code indicates that all components must be entered.

Example

For example, the following set of ED_EXP commands characterises a binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C). It can be used in a POP-file that otherwise only contain experimental information about the ternary system (A-B-C):

```
CREATE_NEW_EQUILIBRIUM 1 0

CHANGE_STATUS COMPONENT A B = ENTERED
```

```
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=1177:10
COMMENT from A-B
```

Using Stability Conditions

Early in the optimization when parameter values are not so good it is often useful to set the driving force for precipitation of a phase (per mole of components) to make sure that it appears where it should. The DGM condition is very useful for making sure that phases appear where they should. It can be removed when the optimization becomes stable.

The DGM condition is also useful for suppressing phases that appear where they should not appear. Do this by setting the value and the uncertainty to something reasonable. For example, the driving force for precipitation of the BCC phase could be set as follows:

```
DGM(BCC)<-0.1:0.1
```

This produces an error even before BCC becomes stable and the weight of the experiment in question can be adjusted as needed. If you specify that the driving force for the BCC phase should be below 0 (DGM(BCC)<0:1E-4 for example), then the optimization converges extremely slowly (if at all). With such a sharp error condition, calculating the equilibrium is like finding the minimum point on a lawn that gently slopes towards a rock wall. The optimization keeps bouncing into the wall.

Another useful stability condition is the phase stability function, abbreviated QF. This can be used to specify that a phase is outside the miscibility gap for a solution phase. If QF(phase) is negative, then the phase is inside the miscibility gap; if QF(phase) is positive, then it is outside the miscibility gap.

Grouping Equilibria with Labels

If you have several equilibria describing experiments that you want to be able to treat collectively, you can give all of the equilibria one and the same label.

Use LABEL to give an equilibrium a label. The label must start with the letter A and can only be up to four characters long. For example, you can insert the following command in several equilibria specifications:

```
LABEL ALH
```

During the optimization, you could use this label to, for example, set all the equilibria that have it to the same weight in the ED_EXP module.

Dividing the POP-File into Several Blocks

For two different reasons, you may have to divide your POP-file into different blocks:

- PARROT uses a buffer for storing compiled experimental data. If there is not enough memory in this buffer for storing all the experiments from the POP-file, then the POP-file can be divided into several blocks. When PARROT encounters the end of a POP-file block, it saves the experimental data that has been compiled to PARROT workspace, clears out the memory buffer and then proceeds to read the next block in the POP-file. This goes on until the experimental data from all the blocks have been saved to the PARROT workspace.

- If you want to put equilibria with different sets of components in one and the same POP-file, then you must divide the file up into blocks. Each block should only contain equilibria that all have the same set of components.

To divide the equilibria in the POP-file into different blocks, enter the *FLUSH_BUFFER* on page 41 command between two equilibria. This command marks the beginning of new block. When the command is encountered during the compilation of the POP-file, the compilation of the current block is terminated, the equilibria saved to the PARROT workspace file and a new block is initiated. That the buffer is reinitiated means that all functions and constants that were entered in the previous block must be entered again in new block in order to be used.

When editing your experimental data in the ED_EXP module, you can select which block to load and edit using *READ_WORKSPACES* on page 160 `<block number>`. The block before the first instance of FLUSH_BUFFER is block number 1, the block after the first instance and before the second instance is block number 2, and so on.

The Setup File

In this section:

Creating the Setup File

The second step is to create the setup file. This is an ordinary Thermo-Calc macro file (*.TCM). Typically, your setup file should contain the following:

- A system definition.
- A section where you enter model parameters and optimizing variables.
- A GO PARROT command.
- A section where initial values are assigned to the optimizing variables for the first optimization cycle.
- A *CREATE_NEW_STORE_FILE* on page 94 `<filename.par>` which creates the PARROT workspace file onto which the results of your optimization are continuously saved and updated. By default this workspace file has the same filename as the setup file, but with the *.PAR filename extension.
- A *COMPILE_EXPERIMENTS* on page 92 `<filename.pop>` command. Since you often encounter syntax errors when you first try to compile a POP-file, it may be useful to execute this command from the console rather than as part of the setup macro file.
- Normally, you also have a *SET_INTERACTIVE* on page 237 at the end of the setup file. This command returns control over Thermo-Calc to the console.

It is possible to interactively execute all these commands one at a time in the console. It may be instructive to enter the commands that would normally go into the setup file interactively while using the on-line help while you are learning to use the PARROT module.

Defining the System

If you have an existing database with information about your system, then you can write the system definition part of your setup file in two different ways.

- If you have an unencrypted user database, then you can define your system by entering DATA module commands directly in the setup file. Use the DATA commands that you normally use to define a system when doing equilibrium calculations in Thermo-Calc Console Mode.
- Define your system by entering DATA module commands directly in the console, then generate a macro file with the GIBBS command *LIST_DATA* on page 77 `<name of setup file>.tcm p` . This command saves all the data that has been loaded in the GIBBS workspace as a macro file. This file can then be modified as required into an optimization setup file.

Creating Additional Composition Sets of a Phase

If you need several composition sets of a phase, then these should be created with the GIBBS command *AMEND_PHASE_DESCRIPTION* on page 52 `<phase name> composition_sets <composition set number>` in the setup file.

If you add composition sets of a phase after the POP-file has been compiled, the data structure in the workspace is corrupted and you have to recompile the POP-file.

Entering the Optimizing Variables

When you have retrieved the data about your system for the setup file, you must manually enter the model parameters that you want to optimize. This is done using the GIBBS command *ENTER_PARAMETER* on page 99, but when you specify the Gibbs energy expression for the parameter, you enter variables that can be given various values into the expression. It is the values of these variables (and thus, the Gibbs energy of the parameter) that you are optimizing.

How you in detail specify the optimizing variables in your set up file depends on which phase you are trying to optimize and what thermodynamic model that is used in the optimization.

Also see *Thermodynamic Models* on page 59 for a range of examples.

Entering Optimizing Variables in Parameter Specifications

There are ninety-nine predefined variables in the PARROT module which you can use in your optimization. These variables are referred to as `V1`, `V2`, `V3`, ... `V98` and `V 99`. When the GIBBS workspace is initialised, all optimizing variables are set to a fixed numerical value of zero. When you do an optimization, there is always some variable for which you want to evaluate the best value, but you can assign fixed values to optimizing variables too. It is often useful to enter all the variables that you can conceivably want to optimize, and then you can interactively select and change which variable to focus at various stages of the optimization.

The setup file excerpts that follow show how optimizing variables are entered. However, before the optimizing variables are introduced in this example, the following command enters an ionic liquid solution phase (a phase for which you have some experimental information):

```
ENTER_PHASE IONIC_LIQ  Y,
AL+3,ZR+4 ; ALO2-1,O-2 ; N N
```

This *ENTER_PHASE* on page 69 command enters a phase called IONIC_LIQ into the GIBBS workspace. This phase is of the type ionic liquid solution, which is specified by type code `Y`. Such a phase is modelled by the *Ionic Two Sublattice Liquid Model*. The next two arguments specify the two sublattices, in this case the cations AL+3,ZR+4 and the anions ALO2-1,O-2. Components that interact in a sublattice are separated by a comma. The first `N` at the end means that no additional constituents are added to the phase. The second `N` means that a list of possible parameters for the phase should not be shown in the console.

There are model parameters that describe the phase which you do not want to optimize, in which case the Gibbs energy expression of the parameter does not contain any optimizing variables.

Example 1

For example, the following parameters of the IONIC_LIQ phase do not contain any optimizing variables:

```
ENTER_PARAMETER G(IONIC_LIQ,AL+3:ALO2-1;0) 298.15 +2*GAL2O3_L; 6000 N

ENTER_PARAMETER G(IONIC_LIQ,AL+3:O-2;0) 298.15 +GAL2O3_L+400000; 6000
N

ENTER_PARAMETER G(IONIC_LIQ,ZR+4:O-2;0) 298.15 +2*GZRO2L; 6000 N
```

These parameters define the Gibbs energy expressions for three constituents in the constituent array, namely AL+3:ALO2-1, AL+3:O-2 and ZR+4:O-2. The names that occur in these expressions—that is, GAL2O3_L and GZRO2L—are the names of complex functions of temperature that are entered in the GIBBS workspace with the *ENTER_SYMBOL* on page 72 command.

The numbers that frame the Gibbs energy expressions specify the temperature range within which the expression should be applied. In the above, the expressions are applied in a temperature range from 298.15 K to 6000 K.

Example 2

In this example, suppose that you want to optimize the model parameter for the ZR+4:ALO2-1 combination, then you could enter the variables V1 and V2 in the Gibbs energy expression for that parameter in the following way:

```
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:ALO2-1;0) 298.15 +GZRO2L +2*GAL2O3_L
+V1+V2*T; 6000 N
```

You normally have different optimizing variables in different parameters, but in some cases you may want several parameters to vary together, in which case you can use the same variable in the Gibbs energy expressions of several parameters.

Entering Interaction Parameters

For some systems, you have to consider interaction parameters in order to take excess Gibbs energy into account and correctly model the phase. By default, the software uses a Redlich-Kister expression for the excess Gibbs energy. The coefficient is entered after the constituent array when you use the *ENTER_PARAMETER* on page 99 command. In the last section, all the parameters were entered with a coefficient of zero (`0`).

Example

To take account of the excess Gibbs energy, you might enter the following:

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;0) 298.15  +V11+V12*T;
6000 N
```

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;1) 298.15  +V13+V14*T;
6000 N

ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;2) 298.15  +V15+V16*T;
6000 N
```

Parameters with interaction coefficients are referred to as *interaction parameters*. The regular parameter has a coefficient of 0. The subregular parameter has a coefficient of 1. It is possible to interaction coefficients up to a value of 9, but you are advised not to use more than three coefficients (that is, with coefficient values of 0, 1 and 2).

Initializing Optimizing Variables in PARROT

Variables that have been entered into Gibbs energy expressions for model parameters in the setup file has to be initialized and given start values before they are optimized.

You have to estimate what start values to give to the optimizing variables based on your knowledge of the system or of relevantly similar systems. There are no general rules for what start values your optimizing variables should have. If you are not able to make any informed estimation about what start values to use, then you may not be able to find a good fit between your experimental data and your calculated results. In this case, it is often best to start the optimization in the so-called alternate mode. In alternate mode, the PARROT module helps you find some reasonable start values for your optimizing variables.

Also see *About Alternate Mode* on page 43.

Even if you are starting your optimization in alternate mode, you still have to initialize the optimizing variables though (you can all give them a start value of 0).

To initialize an optimizing variable and to give it a start value, use either *SET_OPTIMIZING_VARIABLE* on page 114 or *SET_SCALED_VARIABLE* on page 115. Using SET-OPTIMZING_VARIABLE results in a scaling factor equal to the current value of the parameter unless the current value is zero, in which case the scaling factor is 1000. This is typically appropriate for enthalpic parameters, but not necessarily for other parameters. The scaling factor is the factor by which the optimizing variable value is varied during the optimization.

Example

For example, if you want to optimize the variables V1, V2, V11, V13 and V17, then you could enter the following in the setup file:

```
SET_OPTIMIZING_VARIABLE 1 +43000

SET_OPTIMIZING_VARIABLE 2 -35.2

SET_OPTIMIZING_VARIABLE 11 +72000

SET_OPTIMIZING_VARIABLE 13 +27000

SET_OPTIMIZING_VARIABLE 17 -100000
```

The value given to each optimizing variable (+43000 for variable V1 for example) is also that variable's initial scaling factor. If you want to set the initial scaling factor of a variable to a value that is lower or higher than its start value, then use SET-SCALED_VARIABLE `<start value><scaling factor><min value><max value>`.

Creating the Workspace File

In the setup file, after the system definition and the entered optimizing variables, use the PARROT command *CREATE_NEW_STORE_FILE* on page 94 to create and save a PARROT workspace file for the system defined in the setup file. For example, the following command saves all current data on system definitions (elements, species, components, phases), symbol definitions (constants, variables, functions, tables) and parameters that are stored in the workspace used by GIBBS, POLY and PARROT into a file called AL2O3-ZRO2.PAR:

```
CREATE_NEW_STORE_FILE AL2O3-ZRO2
```

The experimental information in the POP-file is not saved to this PARROT workspace file.

Compiling the POP-file

At the end of the setup file, use the command *COMPILE_EXPERIMENTS* on page 92 followed by the name of your POP-file to compile the data in that file and save it to the current PARROT workspace file. Note that you must first have opened or created a new PARROT workspace file before you compile your POP-file. The other argument to the command can typically be given default values with comma signs (,):

```
COMPILE_EXPERIMENTS AL2O3-ZRO2.POP,,,
```

If Thermo-Calc encounters errors in the syntax of the POP-file, then error messages are displayed in the console. Normally, the compilation also stops when syntax errors are encountered. If this happens, then you must correct the errors and recompile the file. It is useful to have two console windows open when you do this. That way, you can use one console for editing the experimental data and another console for compiling and reading any further error messages.

Returning Control to the Console

Put the command *SET_INTERACTIVE* on page 237 at the end of the setup file if you want to return control to the console when the commands in the setup file have all been executed.

Optimizing in PARROT

In this section:

Optimizing the System in PARROT

When you have created a POP-file, a setup macro file and (optionally) EXP-files, you should start doing optimization runs interactively in the console. This process can be divided into a number of steps (such as running optimization, evaluating optimization results, modifying weights and models and adding new information), but usually, you have to go through many optimization cycles before achieving a satisfactory fit between calculation results and experimental data.

Typically, it is not obvious when an optimization is finished. You must exercise your judgement about when the fit you have achieved is good enough.

It is possible to interactively change almost everything in the initial setup macro file and in the POP-file. For example, you can add more parameters to be optimized and modify or add more experimental information.

Changes that Require POP-file Recompilation

Some changes that you do interactively in the PARROT module or the ED_EXP sub-module destroys the data structure in the workspace. For example, if you add more composition sets to a phase, then the number of phases actually change and the links break between the experimental data and the thermodynamic models. Note that if the global minimization technique is used in POLY, then new composition sets that corrupts the PARROT workspace may be created automatically. If this happens, then you have to compile the POP-file again.

If you recompile the POP-file, then the experimental equilibria are calculated with the default start values.

Optimization Workflow

Normally, the workflow during an optimization is the following:

1. In the PARROT module, run the setup macro file using *MACRO_FILE_OPEN* on page 5.
2. Go to ED_EXP with *EDIT_EXPERIMENTS* on page 95, use *READ_WORKSPACES* on page 160 to load your experimental data and then execute *COMPUTE_ALL_EQUILIBRIA* on page 23.
3. If an equilibrium cannot be computed, then this either means that the start values (site fractions, for example) were inappropriate or that the equilibrium cannot be calculated with the current set of parameters. If the latter, then the equilibrium may have to be excluded from the optimization. However, you should make an effort to exclude the possibility that the reason is just that you do not have the appropriate start values for the equilibrium.
4. When each equilibrium is either successfully computed or excluded from the calculation, go back to the PARROT module and run the *OPTIMIZE_VARIABLES* on page 109 command. Give the number of optimization iterations you want the Thermo-Calc

program to carry out as an argument to the command. This number specifies how many different sets of values for the optimizing variables that PARROT tries to fit with the experimental data. It is recommended that you run `0` iterations first to see the discrepancy between the experimental data and the initial calculated results. The current workspace file is automatically updated with the last set of optimized variables and calculated results.

5. List and evaluate the result of the optimization using *LIST_RESULT* on page 104. Typically, what is of interest in the results are the relative standard deviation of the optimizing variables and the error values in the list of calculated experimental data results. If the relative standard deviation for an optimizing variable is very large, this means that the variable doesn't have any effect on the computed results and that the variable should not be used (you can make PARROT ignore the variable by setting its value to `0` with *SET_FIX_VARIABLE* on page 112). If the relative standard deviation is close to zero for a variable, then this might indicate that you need to use more variables. When it comes to errors in the calculated equilibrium results, these can be decreased by lowering the weight that PARROT gives the experiment in the calculation (the more weight, the more the experiment affects the calculated results).
6. Use *OPTIMIZE_VARIABLES* on page 109 or *CONTINUE_OPTIMIZATION* on page 94 to carry out a new optimization cycle. Go back to step 5 above and continue to do optimization cycles until you judge that there is a good enough fit between your calculated results and your experimental data. It is recommended that you do not only rely on feedback from *LIST_RESULT* on page 104 but also frequently plot various diagrams and compare them visually to some of your experimental data.

Ensuring Computation of all Equilibria

When you have run the setup macro file, you should start by trying to compute all the equilibria that were created when your POP-file was compiled. To do this, you must first go to the ED_EXP submodule, and load the experimental data from the current PARROT workspace file with the *READ_WORKSPACES* on page 160`<block #>` command (normally, the block number is `1`).

When you have loaded all equilibria, you should try to compute them all using the ED_EXP command *COMPUTE_ALL_EQUILIBRIA* on page 23. A list of calculated equilibrium results are shown in the console, but the software is not able to reach an equilibrium for an experiment, then the program cancels the calculations and displays an error message.

The following list shows an example output where the first two experiments in the POP-file have been successfully computed, but an equilibrium is not reached for the third experiment. No other equilibria are computed, since the calculations are aborted when the error occurs.

```
Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments

  1 A1    22   1.    2575.3      IONIC_ FLUORI TETR

  2 A1    18   1.    2156.9      IONIC_ CORUND TETR
```

```
*** ERROR  1614 IN QTHISS
*** CONDITIONS CAN NOT BE FULLFILLED
```

When this happens, try to find out why the equilibrium calculation fail. Are the condition start values that you have given the equilibrium inappropriate for example? If you have a similar equilibrium that has already been successfully computed, then you can select the equilibrium that does not work, use the ED_EXP command *SET_ALL_START_VALUES* on page 162 and accept all the suggestions for the site fractions. Alternatively, use *TRANSFER_START_VALUE* on page 34`<equilibrium number>` to make the currently selected equilibrium inherit the start values of the indicated equilibrium. Run *COMPUTE_EQUILIBRIUM* on page 139 again to see if the equilibrium can be computed with the inherited start value.

If you cannot find an explanation of why the equilibrium cannot be computed, then it may be that the experiment is faulty. If so, then this experiment should be excluded from the optimization by being given a weight of 0. You should then runCOMPUTE_EQUILIBRIUM again to make sure that all equilibria can be computed. However, experiments that fail to reach equilibria could succeed in doing so if the optimizing variables have other values. It is therefore sometimes worth trying to include experiments later in the optimization process (when the optimizing variables are relatively close to their final values), even if they had to be excluded at its start. In some cases, it might also be appropriate to change the error tolerance for in an experiment (using the ED_EXP command *EXPERIMENT* on page 24).

You must save the PARROT workspace with *SAVE_WORKSPACES* on page 30 before you exit the ED_EXP module.

Setting Weights

To change the weight of an experiment, first enter the ED_EXP module from PARROT using *EDIT_EXPERIMENTS* on page 95. Then use the *SET_WEIGHT* on page 33 command to set the weight for a specific equilibrium (equilibrium number `3` for example), for a range of equilibria (the equilibria `10-19`) or all the equilibria that have a certain label (such as all the equilibria with the label `A1`). To save the new weight(s), use *SAVE_WORKSPACES* on page 30.

By default, all the experimental information in your POP-file is treated equally: each experiment has a weight of `1`. However, experiments that you excluded because they did not reach equilibrium now have a weight of `0`. The higher the weight of an experiment is, the more Thermo-Calc tries to ensure that the computed result fits the condition measured in that experiment.

The contribution of an experiment’s error to the sum of errors is multiplied by the square of the weight set for that experiment. In other words, if you want to cut the error of an experiment with weight 1.0 by half, then you should use a weight of 0.7. This makes the experiment’s error 0.49. Setting the weight to 1.4 instead makes the error twice as large (1.96).

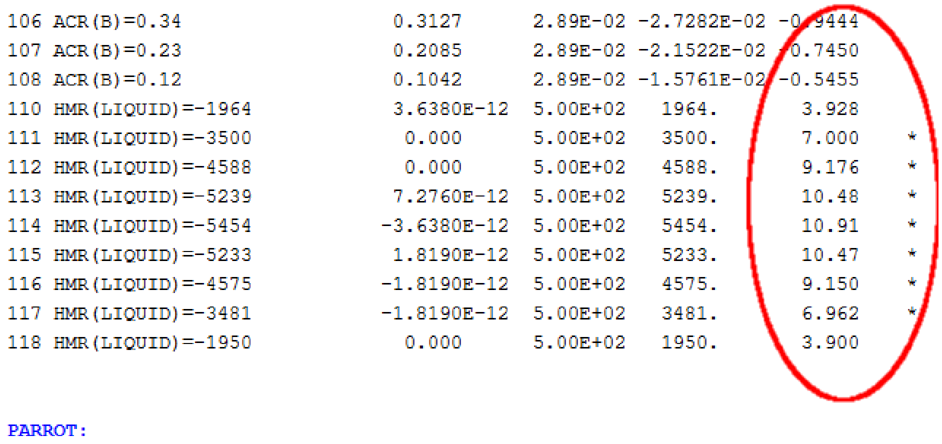
Note that if you use *READ_WORKSPACES* on page 160 after you have changed weights on the experiments, your changes are lost unless you have saved those changes. In the ED_EXP module, you can get a list of all the experiments in the console if you first read the experimental data from the workspace file (with READ_WORKSPACES) and then use *LIST_ALL_EQUILIBRIA* on page 28.

Optimizing and Evaluating Results

When you have ensured that all the experimental data points can reach equilibrium, go back to the PARROT module and use *OPTIMIZE_VARIABLES* on page 109 `<number of iterations>` with `0` iterations. Present the result of this initial optimization by using *LIST_RESULT* on page 104.

When evaluating the optimization results, the most important information is found in the list of experiments at the end of the listed results. The rightmost column shows the difference between the value of the experimental data and the value computed by Thermo-Calc in the last optimization cycle.

The following shows part of list of experiments in the output of a LIST_RESULT command:



```
106 ACR(B)=0.34                 0.3127      2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23                 0.2085      2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12                 0.1042      2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964           3.6380E-12  5.00E+02  1964.        3.928
111 HMR(LIQUID)=-3500            0.000      5.00E+02  3500.        7.000    *
112 HMR(LIQUID)=-4588            0.000      5.00E+02  4588.        9.176    *
113 HMR(LIQUID)=-5239           7.2760E-12  5.00E+02  5239.        10.48    *
114 HMR(LIQUID)=-5454          -3.6380E-12  5.00E+02  5454.        10.91    *
115 HMR(LIQUID)=-5233           1.8190E-12  5.00E+02  5233.        10.47    *
116 HMR(LIQUID)=-4575          -1.8190E-12  5.00E+02  4575.        9.150    *
117 HMR(LIQUID)=-3481          -1.8190E-12  5.00E+02  3481.        6.962    *
118 HMR(LIQUID)=-1950            0.000      5.00E+02  1950.        3.900


PARROT:
```

The experiments for which the optimization has not found a good fit are marked with an asterisk (*) or a hash sign (#) in the rightmost column. An asterisk in this column indicates that the experiment has an error that is larger than the error tolerance and a hash sign indicates that the error is much larger. The error tolerance depends on the degree of accuracy set for that particular piece of experimental information. The error values are presented in the next to rightmost column.

Note that if you are optimizing in *alternate mode*, then you usually do not need to change the weights for the experiments. Instead, you can simply run OPTIMIZE_VARIABLES again, specifying, say, thirty iterations, evaluate the results again, and continue in that way until you are satisfied with the results.

Also see *About Alternate Mode* on page 43.

The Critical Set of Experiments

The set of weighted experiments that you end up with as a result of your optimization is referred to as the *critical set* of experiments. When you work to determine this set and the weights of the experiments, the following factors should be reflected in both the selection of experiments and the weights of those experiments:

- The reliability of the experimental technique.
- The extent of agreement/disagreement between independent measurements of the same quantity.
- The extent of agreement/disagreement between data obtained with different experimental methods.

Continuing the Optimization and Resetting Variables

To continue the optimization after you have used *OPTIMIZE_VARIABLES* on page 109, you can either use this command and enter `<Number of iterations>` again or *CONTINUE_OPTIMIZATION* on page 94 `<Number of iterations>`.

If you use *CONTINUE_OPTIMIZATION* on page 94, then PARROT continues the optimization using the same Hessian matrix. If the optimization is going well but you run out of iterations, then continuing with the same Hessian matrix may be useful.

As before, use *LIST_RESULT* on page 104 to inspect the fit between the calculated and the experimental values for your experiments. If necessary, adjust the weights of the experiments again in the ED_EXP module. You may even discover that you have to exclude additional experiments from the optimization.

Besides looking at the rightmost column in the list of experiments (that is produced when you use LIST_RESULT), it is also useful to look at the *sum of squares* of the errors of all the variables. This is shown in the output of OPTIMIZE_VARIABLES and CONTINUE_OPTIMIZATION. This sum should be as low as possible.

Example Output

The following shows part of the output that you get when using *LIST_RESULT* on page 104:

```
== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1  TO V00

VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
V1      6.94641846E+05    4.30000000E+04    4.30000000E+04    1.42299558E+00
V2     -3.32619842E+02   -3.52000000E+01   -3.52000000E+01    7.91369573E-01
V11     8.37422071E+04    7.20000000E+04    7.20000000E+04    2.02212692E-01
V13     2.65253341E+04    2.70000000E+04    2.70000000E+04    1.45201828E-01
V17    -3.66637428E+05   -1.00000000E+05   -1.00000000E+05    8.04279315E-01

NUMBER OF OPTIMIZING VARIABLES :   5
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM   3.50196879E+05 TO   3.49096720E+05
DEGREES OF FREEDOM   14.  REDUCED SUM OF SQUARES   2.49354800E+04
```

In the example you can see that the sum of squares have decreased slightly. (The final sum of squares that you get after an optimization run is also presented directly in the output from OPTIMIZE_VARIABLES and CONTINUE_OPTIMIZATION.) As long as the sum of squares figure is decreasing, the optimization is working as it should.

When your calculated results have been improving for a while, that is, when the sum of squares has been decreasing, and you are confident that you are making definitive progress, then you should use the PARROT command *RESCALE_VARIABLES* on page 110 to reset the starting values of the optimizing variables to their current values. When you do this, the start values and scaling factors of the optimizing variables (shown in the table's third column in the preceding screen shot), are all set to the current values (shown in the table's second column).

If your optimization is not going well, then you may want to reset the values of your optimization variables to their current start values. To do this, use *RECOVER_VARIABLES* on page 110.

After rescaling the variables, continue the optimization using OPTIMIZE_VARIABLES again. Cycle through calls of the commands OPTIMIZE_VARIABLES/CONTINUE_OPTIMIZATION, CONTINUE_OPTIMIZATION, RESCALE_VARIABLES and OPTIMIZE_VARIABLES again until your set of optimizing variables does not seem to improve anymore. Even when it seems to you that you have reached this point, it is recommended that you use OPTIMIZE_VARIABLES/CONTINUE_OPTIMIZATION a few extra times to make sure that the variable values cannot be further improved, that is, that the sum of squares of the errors of all the variables cannot be reduced further. If the final solution is repeatedly calculated after the same number of iterations and reaching the same result, then it is generally reasonable to accept the current variable values.

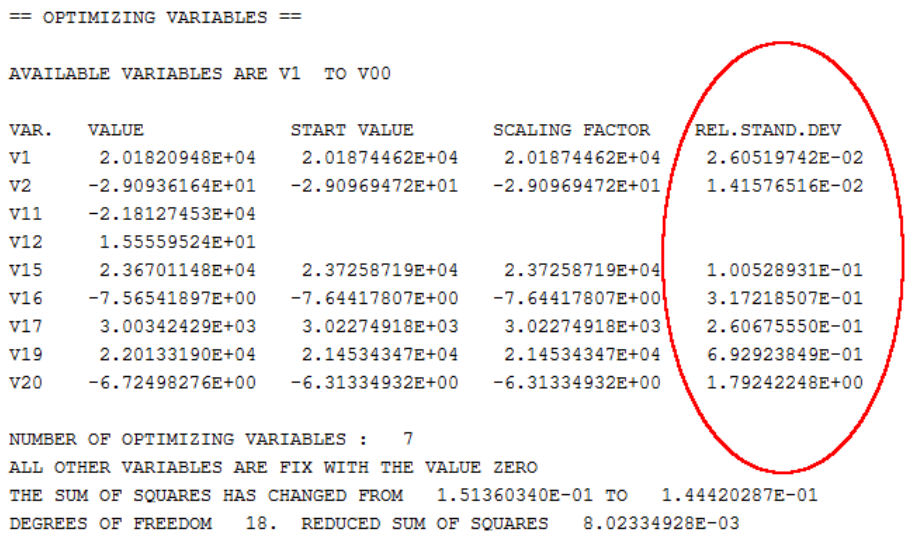
Updating the Set of Optimizing Variables

Besides evaluating the fit between the calculated results and the experimental data, you should also ensure that you have the right number of optimizing variables. If you have too many or too few optimizing variables, then you may not be able to use your model to accurately extrapolate thermodynamic properties in a wide range of temperature, pressure and composition conditions.

With more optimization parameters, the sum of errors usually decrease, but the parameters also tend to become less precisely determined. A measure of this precision is the Relative Standard Deviation (RSD) of each optimizing variable. However, the RSD is only significant if you have used *RESCALE_VARIABLES* on page 110 followed by an optimization which converges and the values of the variables do not change much. The RSD tells you how much the parameter can be changed in either a positive or in a negative direction without changing the reduced sum of errors with more than one unit.

Example

A large RSD value thus means that the parameter has not been determined well.



```
== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1  TO V00

VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
V1      2.01820948E+04    2.01874462E+04    2.01874462E+04    2.60519742E-02
V2     -2.90936164E+01   -2.90969472E+01   -2.90969472E+01    1.41576516E-02
V11    -2.18127453E+04
V12     1.55559524E+01
V15     2.36701148E+04    2.37258719E+04    2.37258719E+04    1.00528931E-01
V16    -7.56541897E+00   -7.64417807E+00   -7.64417807E+00    3.17218507E-01
V17     3.00342429E+03    3.02274918E+03    3.02274918E+03    2.60675550E-01
V19     2.20133190E+04    2.14534347E+04    2.14534347E+04    6.92923849E-01
V20    -6.72498276E+00   -6.31334932E+00   -6.31334932E+00    1.79242248E+00

NUMBER OF OPTIMIZING VARIABLES :   7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM   1.51360340E-01 TO   1.44420287E-01
DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.02334928E-03
```

If such a significant RSD has a value larger than 1, then this typically means that you are using too many optimizing variables. However, the RSD values also depend on the weighting of the experiments, so it is sometimes possible to reduce the RSD by changing weights.

The RSD should not be too low either. If one or more of them is very close to 0, then this suggests that you are trying to optimize the system with too few optimizing variables. You can add optimizing variables interactively using *ENTER_PARAMETER* on page 99 in GIBBS. However, it is recommended that you add a sufficient number of variables in the setup file from the start so that do not need to do this. You can fix variables to a value of 0 until you discover that they are needed.

Besides the RSD, you should also keep an eye on the variable values themselves (shown in the VALUE column, next to the leftmost column in the table shown in the preceding screenshot). If the value of a variable is in the order of 1E5 or higher and this variable has been put in the temperature-independent part of an interaction parameter's Gibbs energy expression, then you may not have the right weights on your experiments or you are using too many optimizing variables. This is also typically the case if a variable with a value in the order of 10 or more (per mole atoms) is in the temperature-dependent part of the Gibbs energy expression of an interaction parameter. Such a high parameter value may lead to inverted miscibility gaps or re-stabilisation of a phase at high temperature. It is important to keep an eye on this since the temperature-independent and the temperature-dependent interaction parameter often varies together. If the temperature-dependent interaction parameter cannot be reliably determined, you may have to fix its value.

Note that even if you have found a good enough fit between calculated and experimental values after an optimization run, a parameter value may suddenly start to change by several orders of magnitude when you use *OPTIMIZE_VARIABLES* on page 109 is used again. If this happens, then careful reconsideration of the weighting of the experiments of the set of optimizing variables is required. However, when the optimization has converged and the parameter values remain stable after repeated use of OPTIMZE_ VARIALBES, this should usually not happen.

Reducing the Number of Optimizing Variables

If you have one or more optimizing variables with RSD larger than 1, then you should remove one or more of the variables by setting them to a value of 0, or alternately, set them to a reliably estimated value (estimated based on, for example, semi-empirical methods).

To fix an optimizing variable to certain value, use the PARROT command *SET_FIX_VARIABLE* on page 112 `<variable number> <value>`.

Plotting Intermediate Results

It is typically not sufficient to look at the plain text output of *LIST_RESULT* on page 104 to reliably judge how the optimization is progressing. Plotting a phase or property diagram of the system you are optimizing using the POLY and POST modules is often very useful.

It is recommended that you create a macro file for plotting the diagram since you probably want to repeatedly plot the diagram as you progress with the optimization. This macro file can then be called directly from the PARROT module with the *MACRO_FILE_OPEN* on page 5 command.

Superimposing Experimental Data from EXP-files

If you create one or several EXP-files based on the experiments in your POP-file, you can visually compare the fit your plot and the experimental data you are optimizing the system against. An EXP-file contains data points specified in the DATAPLOT format. You could make an EXP-file for each type of data that you are using in the optimization.

Use the POST command *APPEND_EXPERIMENTAL_DATA* on page 192 to superimpose the data points in an EXP-file on a phase or property diagram that you have plotted. For example, to put the experimental data points from a file entitled DP.EXP onto a plotted diagram, you could enter the following:

```
APPEND_EXPERIMENTAL_DATA Y DP.EXP 0 1
```

Such a command call tells Thermo-Calc to superimpose the data points in dataset 1 of DP.EXP onto the plot in the Console Results window, but not to impose any information about axis scaling, labels and other information which is normally found in the prologue of the DP.EXP file.

The POST command *QUICK_EXPERIMENTAL_PLOT* on page 201 can also be used to superimpose data points on a plotted phase or property diagram.

Also see the *DATPLOT User Guide* included with this documentation set.

Finalizing the Optimization

In this section:

Finishing the Optimization

When to stop optimizing is a matter of judgement. It is rarely the case that you finish optimizing a system with the feeling that it cannot be improved.

The final step is to update your files with the final results. Besides updating your database file (or alternatively, creating a new database file), it is advised that you also update your setup and POP-files with the final weights and optimizing variable values.

Rounding off Optimizing Variable Values

When you save the optimizing variable values, it is important that you round off the values correctly. When you have a metallic system, it is usually best to keep whatever number of decimal digits that you need to make less than one J/mol difference at 1000 K. When you have an aqueous system or a system that you are optimizing based on data from very different temperature ranges, then this is not always the only appropriate guideline. However, rounding off the values in such a way that it gives a difference that is larger than one J/mol may lead to differences in the phase diagram.

Another approach you can take when rounding off variable values is by progressively fixing the value of more and more of the variables. This allows you to round-off all but one of the variables values so that each only has a few significant digits. Variables whose values have been rounded off in this way are easier to handle compared with those that that are rounded off so that they continue to have many significant (non-zero) digits.

To round off the variable values according to this second approach, first use *SET_FIX_VARIABLE* on page 112 to set the variable(s) with the highest RSD to a rounded off value (such as, say, 0.4). When you then re-optimize using *OPTIMIZE_VARIABLES* on page 109, the sum or errors changes. However, you should get almost exactly the same sum of errors as before after you rescale the variable values using *RESCALE_VARIABLES* on page 110. (If the sum of errors is different, then this means that the variable with the highest RSD was not rounded off in a good way.) If you successfully round off the first variable value, then continue to round of the optimizing variable which now has the highest RSD. Continue doing this until you have fixed all but one of the optimizing variables to their rounded-off values. The final sum of errors that you get after having fixed the variable values should not deviate significantly from the initial sum of errors you had before starting to round-off the variable values.

Updating the Database File

To update the database file (with filename extension TDB) open it in a text editor and enter or update each of the parameters that you have optimized.

For example, suppose you have the following command in your setup file:

```
ENTER_PARAMETER L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15  +V17; 6000 N
```

If you then end up with a value for optimizing variable V17 of -100000, then you should enter the following under the IONIC_LIQ phase in the database file:

```
PARAM L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15 -100000; 6000 N REF !
```

If you often need to round-off the optimizing variable value in some way, see *Rounding off Optimizing Variable Values* on the previous page.

When you have updated or entered the parameters that you optimized, save the database file.

Creating a Database File

In some circumstances you may want to save all the information about your system into a new database file. To do this, go to the GIBBS module and use LIST_DATA `<Filename> N`. This creates a new user database file that contains all the information about the system that is in the workspace.

The N-argument tells the *LIST_DATA* on page 77 command to save the output into database file rather than some other type of file, such as a macro file for example. Note that the output database file that you get from LIST_DATA have to undergo some manual editing before it can be used as proper database file.

Updating the Setup File and the POP-file

It may be useful for you to be able to recreate your optimization from scratch. It is therefore recommended that you do the following when you are done with the optimization:

- Update your POP-file so that it contains the weights of your critical set of experiments. Use *SET_WEIGHT* on page 33 to set the weights directly in the POP-file. You may also have to use *SET_START_VALUE* on page 171 for some conditions in the POP-file. Otherwise, you may not be able to compute the equilibria with *COMPUTE_ALL_EQUILIBRIA* on page 23.
- Copy the final values of your optimizing variables and set them as start values of the variables in the setup macro file (with *SET_FIX_VARIABLE* on page 112).

It is important that you round off the values of the optimizing variables correctly. See *Rounding off Optimizing Variable Values* on the previous page. When you have done this, you can run the setup macro file to recreate the final result of the optimization.

Alternate Mode

In this section:

About Alternate Mode

To turn Alternate Mode ON or OFF, use the PARROT command *SET_ALTERNATE_MODE* on page 111.

When you have one or more multi-phase equilibria (that is, with the fixed phase-status) in your POP-file and the optimizing values lack appropriate starting values (such as the default value of 0 for example), then Thermo-Calc may not be able to compute the equilibria for the experiments. In these cases, a common tangent cannot be found, that is, a state where the chemical potentials for all components are the same in all phases cannot be found. A common tangent may not exist or it be found at the wrong composition or temperature given the initial set of model parameters.

If you are not able to estimate reasonable starting values for the optimizing variables, then this problem can be overcome by initially running your optimization in alternate mode. The alternate mode in PARROT module should help you find reasonable starting values for the optimizing variables. Note that you are only supposed to use alternate mode in the beginning of the optimization. Once you have achieved a reasonable fit between calculated results and experimental data, turn off alternate mode and calculate all equilibria again in the normal mode.

In alternate mode, PARROT modifies multi-phase equilibria so that the chemical potentials for each stable phases is calculated separately. For example, consider the following experimental equilibrium:

```
CREATE_NEW_EQUILIBRIUM 1 1

CHANGE_STATUS PHASE LIQ FCC=FIX 1

SET_CONDITION T=1000 P=1E5

EXPERIMENT X(LIQ,B)=.2:.01 X(FCC,B)=.1
```

When PARROT optimizes in alternate mode, the computation of this equilibrium is done by way of the following two calculations:

```
CHANGE_STATUS PHASE LIQ=FIX 1

SET_CONDITION T=1000 P=1E5 X(LIQ,B)=.2

CHANGE_STATUS PHASE FCC=FIX 1

SET_CONDITION T=1000 P=1E5 X(FCC,B)=.1
```

The difference between the chemical potentials in every pair of phases is calculated and PARROT tries to adjust the parameters of the phases so that these differences are minimized. In other words, PARROT tries to make the chemical potentials equal in all phases. For PARROT to be able to do this, some additional information about the experimental multi-phase equilibria is required, at least for all invariant equilibria.

Optimizing in Alternate Mode

When you are optimizing in the alternate mode, you usually do not need to enter the ED_EXP module and manually change the weights of experiments that the computed results have not been fitted well with. Instead, after using *OPTIMIZE_VARIABLES* on page 109 initially with no iterations, and listing the result with *LIST_RESULT* on page 104, simply run OPTIMIZE_VARIABLES again specifying, say, thirty iterations. Continue to optimize until your optimization seems to be going in the right direction, then set the optimizing variables' starting values to their current values use *RESCALE_VARIABLES* on page 110 before you turn alternate mode off by answering N at the *SET_ALTERNATE_MODE* on page 111 prompt.

Preparing the POP-file for Alternate Mode

Information in your POP-file that concerns equilibria with ENTERED or DORMANT phases is ignored when you optimize in alternate mode.

To use the alternate mode, ensure that there is enough information about each phase in a given equilibrium. In addition to the temperature and pressure of the system, you should specify the composition of all phases in a given equilibrium. This is done with, *SET_CONDITION* on page 165, *EXPERIMENT* on page 24or *SET_ALTERNATE_CONDITION* on page 30.

If both compositions of a binary tie-line have been measured, then you could specify this in the POP-file in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1

CHANGE_STATUS PHASE FCC BCC=FIX 1

SET_CONDITION P=1E5 T=1000

EXPERIMENT X(BCC,B)=.2:.01 X(FCC,B)=.3:.01
```

This equilibrium could be calculated with alternate mode without any modification. The compositions specified with the experiment command is used as condition when the thermodynamic properties of each phase are calculated.

Examples of SET_ALTERNATE_CONDITION

The following topics demonstrate how *SET_ALTERNATE_CONDITION* on page 30 is used to prepare different kinds of equilibria for optimization in alternate mode.

Specifying the Composition of One Side of a Binary Tie-Line

If only one side of the tie-line has been measured, then you must provide an estimate of the composition of the other phase. You can make such an estimate with SET_ALTERNATE_CONDITION. This command has no effect unless alternate mode is turned on. The equilibrium described could thus be specified in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC=FIX 1
SET_CONDITION P=1E5 T=1000
EXPERIMENT X(BCC,B)=.2:.01
SET_ALTERNATE_CONDITION X(FCC,B)=.3
```

When the alternate mode is turned on, the composition given by the SET_ALTERNATE_CONDITION command is used for the FCC phase. The properties of the BCC phase is calculated using the composition specified by experiment as a condition.

Specifying the Compositions of a Three-Phase Equilibrium

If you have a three-phase equilibrium in your POP-file, then one of its compositions can be specified as experimentally determined, while two can be provided as alternate conditions:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=912:5 X(LIQ,B)=0.2:.02
SET_ALTERNATE_CONDITION X(FCC,B)=0.1 X(BCC,B)=.4
```

Specifying the Composition of a Stoichiometric Phase

When you specify the composition of stoichiometric phase with SET_ALTERNATE_CONDITION, the value must be given with at least seven decimal digits, as in the following example:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQ A2B=FIX 1
SET_CONDITION P=1E5 X(LIQ,B)=0.2
EXPERIMENT T=992:5
SET_ALTERNATE_CONDITION X(A2B,B)=.6666667
```

Entering Other Experiments in the POP with Alternate Mode

The following table shows some additional examples of how to enter different kinds of experiments in the POP-file when you are using the alternate mode.

Example	**ED_EXP commands**
Two-phase equilibrium: The melting temperature of an Au-Cu alloy	CHANGE_STATUS PHASE LIQUID FCC=FIX 1 SET_CONDITION X (FCC,CU)=0.14 P=1E5 EXPERIMENT T=970:2 SET_ALTERNATE_CONDITION X(LIQUID,CU)=0.16
Invariant equilibrium experiment: A three-phase equilibrium in a binary system	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1 SET_CONDITION P=1E5 EXPERIMENT T=912:5 SET_ALTERNATE_CONDITION X(FCC,B)=0.1SET_ ALTERNATE_CONDITION X(BCC,B)=0.4SET_ALTERNATE_CONDITION X (LIQ,B)=0.2
Ternary system, with two compositions measured (both with uncertainty 0.02)	CREATE_NEW_EQUILIBRUM 1 1 CHANGE_STATUS PHASE FCC BCC=FIX 1 SET_CONDITION T=1273 P=1E5 SET_CONDITION X(FCC,B)=0.1:0.02 EXPERIMENT X(FCC,C)=0.12:.02 SET_ALTERNATE_CONDITION X (BCC,B)=0.17 SET_ALTERNATE_CONDITION X(BCC,C)=0.07

Troubleshooting

During an optimization, you are likely to run into many different problems and challenges. This topic gives some general guidelines that can help avoid common mistakes and problems.

In this section:

Useful Guidelines

The following rules of thumb are generally good to adhere to when you are planning and executing an optimization:

- Do not use data from thermochemical tables of unknown origin.
- Use experimentally determined properties; avoid converted quantities.
- Carefully estimate the accuracy of the experiments.
- Correct systematic errors (by adjusting a temperature scale for example).
- Use negative information such as, for example, the information that a phase should not be stable in a composition or temperature region.
- With a hundred activity measurements in a system but only ten composition points from the phase diagram, it is often appropriate to decrease the weights on the activity experiments.
- If you initially exclude any intermediate phases to only optimize the liquid and the terminal or end-member phases for the pure components, then it is often useful to compute a metastable phase diagram with just these phases. In the metastable phase diagram, the metastable solubility lines should not have any strange kinks or turns. Such a diagram is often also useful to compute at later stages in the optimization.
- When you have fitted the liquid phase and some solution phases reasonably well, then you can fix the optimizing variables that characterise these phases. You can then go on and optimize the variables for the intermediate phases.
- Phases with miscibility gaps are always difficult to optimize. Try to keep control of the miscibility gaps by using real or estimated experimental information. (Note that it is not possible to calculate the top of a miscibility gap as a single equilibrium.)
- Phases with order/disorder transformation are often difficult to optimize. It may be difficult to find the right start values on the optimizing variables. The TABULATION module (see *TABULATION_REACTION Commands* on page 247) can be useful sometimes. Properties for specified site fractions can be calculated in the TABULATION module. This is not possible in the POLY module since this module only calculates for equilibrium site fractions. The ordered state may also disappear during the optimization of these phases. If this happens, you may be able to add an experiment that controls the state of order.
- Only use the alternate mode to find an initial set of model parameters that can then be make it possible to calculate the experimental equilibria in the normal mode.
- When you have achieved a satisfactory fit between calculated results and experimental data with an appropriate number of optimization variables, perform a couple of final optimization runs to make sure that your results are stable.

- Make sure that the values of the optimizing variables keep within a reasonable range. If a variable starts to change several orders of magnitudes, then you must consider whether you have the right weights on the experiments and whether you are using too many optimizing variables.

Excluding and Including the Correct Equilibria

Use as few experiments as possible initially to get a reasonable overall fit. It is generally best to first focus on the invariant equilibria, as well as metastable states that can be estimated by excluding some phases. Crucially, any experiments for which the computed results are clearly faulty should be excluded from the final critical set, while all important invariant equilibria are calculated and included in this critical set.

If you cannot compute some invariant equilibria with intermediate phases, then it may be best to first exclude those phases from the optimization and only optimize the liquid and the most important solution phases. After you have obtained reasonable results for these phases, you can enter the intermediate phases back in again. With the variables for the optimized liquid and solid phases set fixed, you can finally optimize the intermediate phases.

Conflicting Data

It is important that you do not include conflicting sets of data at the same time during an optimization. After all, if they are genuinely conflicting, then at least one of the sets must be incorrect. If you have conflicting sets of data, then only use one of these sets at a time together with the rest of the data. Often, the optimization makes it clear which dataset coheres best with the other information that is available about the system.

Sometimes, conflicting data cannot be detected directly. For example, you may have activity data which is inconsistent with solubility data from the phase diagram. This would be indicated by large errors in the fit when both the activity data and the solubility data are included. To find these inconsistencies, let alone correct the errors, you may thus have to optimize with some datasets excluded.

Experiments and Experimental Data

These topics contain examples of different kinds of equilibria in different kinds of systems. They are intended to help you figure out how to use various kinds of experimental data when creating POP-files. The topics that follow contain examples how to enter various kinds of experimental data into a POP-file.

In this section:

Phase Diagram Data

P-T-X phase diagram data for binary and ternary systems, or systems of even higher order can be used in the POP-file. This includes data of the following types:

- Data about the temperature- and composition-dependence of various properties (obtained from differential thermal analysis (DTA) measurements for example), including enthalpy, lattice parameter, dilatometric length, electronic conductivity and magnetic susceptibility;
- Data about reaction types (invariant/monovariant) and phase relations obtained from qualitative or quantitative metallographic studies;
- Data about phase amounts or compositions obtained from microprobe measurements (using X-ray spectroscopy or transmission electron microscopy (TEM));
- Data about the positions or directions of two-phase tie-lines and three-phase equilibria for ternary systems.

Example

The following table shows a POP-file excerpt that demonstrates how some kinds of phase diagram data can be entered:

Example	**ED_EXP commands**

Solidus (melting temperature) of an Au-Cu alloy	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE LIQUID FCC=FIX 1`
	`SET_CONDITION X(FCC,CU)=0.14 P=1E5`
	`EXPERIMENT T=970:2`

Three-phase equilibrium in a binary A-B system	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1`
	`SET_CONDITION P=1E5`
	`EXPERIMENT T=912:5`

Congruent transformation in a binary A-B system	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE BCC LIQUID=FIX 1`
	`SET_CONDITION P=1E5 X(BCC,B)-X(LIQ,B)=0`
	`EXPERIMENT T=1213:10`

Tie-line in a ternary A-B-C system	An uncertainty factor is set not only for the experimental measurement, but also for the X(FCC,B) condition. The factor is 0.02. `CREATE_NEW_EQUILIBRUM 1 1`

Example	ED_EXP commands
	CHANGE_STATUS PHASE FCC BCC=FIX 1 SET_CONDITION T=1273 P=1E5 X(FCC,B)=0.1:0.02 EXPERIMENT X(FCC,C)=0.12:.02

Data for Individual Compounds

You can use data about individual components in the POP-file. Such data includes activity, heat capacity, heat content, entropy, Gibbs energy of phase transformations, heat of transition and heat of melting.

Examples

Example	ED_EXP commands
Carbon activity data in the fcc phase	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=FIX 1 CHANGE_STATUS PHASE GRAPHITE=D SET_REFERENCE_STATE C GRAPHITE,,,, SET_CONDITION P=101325 T=1273 X(MN)=0.03 SET_CONDITION X(C)=0.03 EXPERIMENT ACR(C)=0.29:5%
Ln(activity coefficient for O)	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE IONIC_LIQ=FIX 1 CHANGE_STATUS PHASE GAS=D SET_CONDITION X(O)=0.02 T=1523 P=101325 SET_REFERENCE_STATE O GAS,,,, ENTER_SYMBOL FUNCTION LNFO=LOG(ACR(O)/X(O)); EXPERIMENT LNFO=-1.5:0.01
Entropy at 298.15 K of Cu2O	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE CU2O=FIX 1 CHANGE_STATUS PHASE CUO=FIX 0 SET_CONDITION P=101325 T=298.15 EXPERIMENT S=92.36:1
Gibbs energy of formation of NiAl2O4	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 CHANGE_STATUS PHASE FCC O2GAS=DORM

Example	ED_EXP commands
	SET_REFERENCE_STATE NI FCC,,,, SET_REFERENCE_STATE AL FCC,,,, SET_REFERENCE_STATE O O2GAS,,,, SET_CONDITION P=101325 T=1000 N(NI)=1 N(AL)=2 SET_CONDITION N(O)=4 EXPERIMENT GM=-298911:5%
Heat capacity of MgFe2O4	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(FE)=2 N(MG)=1 N(O)=4 SET_CONDITION T=800 ENTER_SYMBOL FUNCTION CP=H.T; EXPERIMENT CP=207:5%
Heat content (H-H298) for MnFe2O4	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 T=298.15 N(MN)=1 N(FE)=2 SET_CONDITION N(O)=4 ENTER_SYMBOL VAR H298=H; ENTER_SYMBOL FUN HMNFE2O4=H-H298; CREATE_NEW_EQUILIBRIUM 2 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(MN)=1 N(FE)=2 N(O)=4 SET_CONDITION T=400 EXPERIMENT HMNFE2O4=16610:5%

Single Phase Mixing Enthalpies or Partial Enthalpies

You can use calorimetric data for mixing in the POP-file. This data could be the result of, for example, drop calorimetry or scanning calorimetry. This includes data about, for example, enthalpy of mixing of liquids, series of mixing-enthalpy and about partial enthalpy. Information about enthalpies of mixing can also be derived from theoretical principles using special quasi-random structures (SQSs).

Example

Example	ED_EXP commands

Enthalpy of mixing in the liquid state of an Au-Cu alloy	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE LIQUID=FIX 1`
	`SET_CONDITION T=1379 P=1E5`
	`SET_CONDITION X(LIQUID,AU)=0.0563`
	`SET_REFERENCE_STATE AU LIQ * 1E5`
	`SET_REFERENCE_STATE CU LIQ * 1E5`
	`EXPERIMENT HMR=-1520:200`

Enthalpies of Formation and Enthalpies of Reactions

You can use calorimetric data for phase transformations in the POP-file. This data could be the result of, for example, direct-reaction calorimetry, solution calorimetry or combustion calorimetry. Information about enthalpies of formation can also be derived from theoretical principles.

Examples

Example	ED_EXP commands

Enthalpy of melting of the eutectic in the Al2O3-ZrO2 binary (J/g)	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE CORUNDUM ZRO2_TETR=FIX 0`
	`CHANGE_STATUS PHASE IONIC_LIQ=ENT 1`
	`SET_CONDITION P=101325 N=1 LNAC(O)=-80`
	`SET_REFERENCE_STATE ZRO2 TETR,,,,,,`
	`SET_REFERENCE_STATE AL2O3 CORUND,,,,,,`
	`EXPERIMENT HWR=1080:90`

Enthalpy of formation of o-CaZrO3 from the component oxides	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE ZRO2_MONO HALITE CAZRO3_O=ENT 1`
	`SET_CONDITION T=298.15 P=101325 N(CAO)=.5`
	`SET_CONDITION N(ZRO2)=.5 LNAC(O)=-20`
	`SET_REFERENCE_STATE CAO HALITE,,,,`
	`SET_REFERENCE_STATE ZRO2 ZRO2_MONO,,,,`
	`EXPERIMENT HMR(CAZRO3_O)=-15960:5%`

Chemical Potentials via EMF Measurements

You can use chemical potentials and activities/activity coefficients from electromagnetic field (EMF) measurements in the POP-file.

Example

Example	ED_EXP commands

Emf data on Cu(s)/Cu2O (s)	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC CU2O=FIX 1`
	`CHANGE_STATUS PHASE O2GAS=DORM`
	`SET_CONDITION P=101325 T=1000`
	`SET_REFERENCE_STATE O O2GAS,, 100000`
	`EXPERIMENT MUR(O)=-95387:1000`

Driving Force for Metastable Phases

You can use chemical driving forces for metastable phases in the POP-file.

Examples

Example	ED_EXP commands
To prevent BCC_A2 to be stable	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1 M7C3 M23C6=FIX 1 CHANGE_STATUS PHASE BCC_A2=D SET_CONDITION P=101325 T=1473 EXPERIMENT DGM(BCC)<-0.1:0.1
To promote CEMENTITE to be stable	CHANGE_STATUS PHASE BCC M7C3 GRAPHITE=FIX 1 CHANGE_STATUS PHASE CEMENTITE=DORMANT SET_CONDITION P=P0 T=973 EXPERIMENT DGM(CEM)>0.1:0.01

Pressure-Temperature-Volume EOS Data

You can use Pressure-Temperature-Volume Equation of State (EOS) data in the POP-file. Such data includes, for example, molar volume, density, thermal expansion and bulk-modulus/compressibility.

Examples

Example	ED_EXP commands
Volume of liquid Pt	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID=ENT 1 SET_CONDITION P=101325 N=1 T=1873 EXPERIMENT VM=1.00758E-5:5%
Thermal expansion	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=ENT 1 SET_CONDITION P=101325 N=1 T=400 ENTER_SYMBOL FUNCTION ALPHA=VM.T/VM/3; EXPERIMENT ALPHA=2.35E-5:5%

Crystal Structure, Lattice Parameters and Site-Occupancy

You use information about defects, ordering or site occupancy, as well as information about crystal structures in the form of lattice parameter values. This information may come from measurements made by X-ray, neutron diffraction, Mössbauer spectroscopy or perturbed angular-correlation.

Examples

Example	**ED_EXP commands**

Lattice parameter for fcc	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC_A1=ENT 1`
	`SET_CONDITION P=101325 N=1 T=298.15`
	`SET_CONDITION X(CR)=0.05`
	`ENTER_SYMBOL FUNCTION LPFCC=((4*VM/6.02214179E23)**(1/3))*1E10;`
	`EXPERIMENT LPFCC=4.02:5%`

Lattice parameter for bcc	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE BCC_A2=ENT 1`
	`SET_CONDITION P=101325 N=1 T=298.15`
	`SET_CONDITION X(AL)=0.08`
	`ENTER_SYMBOL FUNCTION LPBCC=((2*VM/6.02214179E23)**(1/3))*1E10;`
	`EXPERIMENT LPBCC=2.90:5%`

Site-occupancy, degree of inversion for spinel	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE SPINEL=ENT 1`
	`SET_CONDITION P=101325 N(MG)=1 N(AL)=2 N(O)=4`
	`SET_CONDITION T=1073`
	`EXPERIMENT Y(SPINEL,AL+3#1)=0.31:5%`

Magnetism and Other Atomistic Properties

You can use data about atomistic properties such as magnetism and Curie temperatures in the POP-file.

Example

Example	**ED_EXP commands**

Curie temperature of MnxFe3-xO4, x=1.26	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE SPINEL=ENT 1`
	`SET_CONDITION  T=520 P=101325 N(O)=4`
	`SET_CONDITION N(FE)+N(MN)=3 N(MN)=1.26`
	`EXPERIMENT TC(SPINEL)=520:5`

Data About Systems of Different Orders

You might want to use data about systems of different orders in the same optimization, such as data about a binary equilibrium with components A and B in a ternary system with components A, B and C, together with data about equilibria in the binary system with components A and B. To do this, you must first suspend all components in the ternary system (A, B and C), and then set the two components you want binary information on (A and B) to status `ENTERED`.

Suspending all components is done by giving the initialization code 0 to the *CREATE_NEW_EQUILIBRIUM* on page 143 command. The components about which you want to use binary information must then be entered again using the *CHANGE_STATUS* on page 59 command.

Example

Example	**ED_EXP commands**

A binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C)	`CREATE_NEW_EQUILIBRIUM 1 0`
	`CHANGE_STATUS COMPONENT A B = ENTERED`
	`CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1`
	`SET_CONDITION P=1E5`
	`EXPERIMENT T=1177:10`

Thermodynamic Models

The most common models used in assessments are described briefly in these topics. Examples of how to write the phase definitions in the setup-file are also given for each of these models. In addition to the models described here, a large number of thermodynamic models for various phases in different states have been implemented.

In this section:

Gas

The gaseous mixture phase is usually treated as a substitutional phase without sublattice. In the gaseous mixture phase, there are usually molecules formed, and the number of constituents of the gas phase is often much larger than the number of elements. These complex constituents have to be defined as species. The ideal gas model may handle a gas phase under low pressures (and low temperatures). This implies that the P-V-T relations and thermodynamic properties of pure gaseous species are calculated as for ideal gas, and that there is interaction between gaseous species in the mixture. In a defined system, there may only exist one gaseous mixture phase. Type code `G` is used for the gas phase:

```
ENTER_PHASE GAS G, 1 H,H1O1,H1O2,H2,H2O1,H2O2,O,O2,O3; N N
```

Compound Energy Formalism

If the atoms are sufficiently different in size, electronegativity or charge, they may prefer different types of sites in the lattice of crystalline solids. In some cases, a solute atom may even occupy interstitial sites between the normal lattice sites. All such phenomena are treated in Thermo-Calc by the sublattice concept. The Compound Energy Formalism (CEF) has proved to be the most general formalism for many different types of solution phases. It is therefore by default applied to various solid solution phases in the Thermo-Calc software package. CEF can also take ionic constraints (charged cation/anion species) into account. For a comprehensive description on the CEF, please see Hillert (2001), Frisk and Selleby (2001), Sundman and Ågren (1981).

Since the CEF is used by default, no special notation is needed in the phase definition, except for ionic phases, where type code `I` is given.

Examples

Examples of phase definitions in a setup-file using the CEF:

```
ENTER_PHASE SPINEL I, 4 1 2 2 4

     FE+2,FE+3; FE+2,FE+3,VA; FE+2,VA; O-2; N N

ENTER_PHASE SIGMA, 3 10 4 16

     AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; N N

ENTER_PHASE FCC_A1, 2 1 1

     CR,FE,MN; C,N,VA; N N

ENTER_PHASE BCC_A2, 2 1 3

     CR,FE,MN,VA; C,N,VA; N N
```

Substitutional Liquid

The liquid phase is normally (but not always) modelled as a substitutional phase with no sublattice, which is occupied by two or more constituents. The constituents are normally the elements, but molecules or associates can also be used. Type code `L` is used for the liquid phase.

Example

```
ENTER_PHASE LIQUID L, 1
```

```
          AL,C,CR,FE,MO,NI,SI ;  N N
     ENTER_PHASE LIQUID L, 1
          C,FE,FEO,FEO3/2,NI,NIO ;  N N
```

Ionic Two-Sublattice Liquid Model

Within the framework of the CEF, the ionic two-sublattice liquid (I2SL) model was developed to be used when there is a tendency for ionization in the liquid, which happens in liquid oxides and sulphides for example. The same model can be used both for metallic and oxide melts. At low levels of oxygen, the model becomes equivalent to a substitutional solution model between metallic atoms. Two sublattices are assumed, one containing charged cations and one containing charged anions, neutrals and vacancies. The complication for an ionic liquid is that the numbers of sites on the cation sublattice and anion sublattice vary with the composition to preserve electroneutrality. For a comprehensive description on the I2SL model, see Hillert et al. (1985), Sundman (1991). In these references, the possible excess parameters are also discussed. Type code `Y` is used for the I2SL model.

Example

Examples of phase definitions in a setup-file:

```
     ENTER_PHASE LIQUID Y,
          AL+3,CR+2,FE+2,NI+2; VA; N N
     ENTER_PHASE IONIC_LIQ Y,
          CA+2,MG+2; O-2; N N
     ENTER_PHASE IONIC_LIQ Y,
          AL+3,CA+2,FE+2,MG+2,SI+4;
          ALO2-1,O-2,SIO4-4,VA,FEO3/2,SIO2; N N
```

Models for Ordered Phases

Some solution phases have chemical order-disorder transformations: for example, the disordered FCC_A1 phase can transform to the ordered $L1_2$ or $L1_0$ structure where the atoms of different kinds occupy different sublattices. In some cases, it may be advantageous and easy to describe such ordered structures as completely different phases; but in some other cases, like the B2-ordered BCC structure in Al-Fe, the disordered and ordered structures must be described as one singe phase because the transformation is of second order along a line in temperature and composition.

The ordering can easily be described by the CEF. For instance, an ordered FCC phase with only $L1_2$ or $L1_0$ ordering can be efficiently handled by the so-called Two Substitutional-Sublattice Ordering Model (2SL model), while an ordered FCC with both $L1_2$ and $L1_0$ ordering must be described with four sublattices using the so-called Four Substitutional-Sublattice Ordering Model (4SL model). Please note that in both these models, all the substitutional constituents must enter into these sublattices. In addition, you may also have one sublattice for interstitials.

Thermo-Calc supports a feature of splitting the parameters of a chemically ordered phase onto two different phase descriptions. This is very convenient. In this way, you can have one phase for all parameters describing the disordered state (the configuration independent state) and in the other phase only those parameters needed to describe the remaining part (the configuration dependent part), that is, the Gibbs energy contribution due to the ordering transformation. This has been implemented in such a way that the contribution from the configuration dependent part is zero when the solution phase is disordered. The optimization of the disordered phase is independent of the order-disorder transformation; the ordering energy is an add-on to the disordered part. This is particularly useful in higher order systems, as an ordered phase can dissolve several elements that have no particular contribution to the actual ordering. The phases Gibbs energy add together by giving this command in the setup-file: *AMEND_PHASE_DESCRIPTION* on page 52 `<ordered phase> disordered_part <disordered phase>`

Since PARROT does not automatically create new composition sets, it is necessary to create composition sets for both the ordered and disordered phases in the setup-file: `Amend_phase_description <phase> composition_sets <new highest set number>,,,,`

Example

Example of phase definitions for the corresponding disordered and ordered parts in a setup-file:

```
ENTER_PHASE FCC_A1, 2 1 1

     AL,CR,FE,NI; VA; N N

ENTER_PHASE FCC_L12, 3 .75 .25 1

     AL,CR,FE,NI ; AL,CR,FE,NI; VA; N N

AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_A1
```

4SL Model for FCC, HCP and BCC

Ordered FCC, HCP and BCC solution phases handled by the 4SL model requires four sublattices for substitutional ordering and can additionally have an interstitial sublattice. A 4SL model is especially useful for modelling different kinds of ordered phases that are based on the same disordered phase, such as $L1_0$ and $L1_2$ based on FCC_A1, and B2, $D0_3$, $L2_1$ and B32 based on BCC_A2 etc.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours. These corners are equivalent lattice points, thus all G parameters for each end-member with the same elements, but distributed on different sites, must be identical. It should be emphasized that the end-member energy here represents the ordering energy rather than the formation energy of the compound.

The constraints on the parameters in the 4SL model can be derived based on the symmetry of the lattice:

$G_{A:B:B:B}=G_{B:A:B:B}=G_{B:B:A:B}=G_{B:B:B:A}$

$G_{A:A:B:B}=G_{A:B:A:B}=G_{A:B:B:A}=G_{B:A:A:B}=G_{B:A:B:A}=G_{B:B:A:A}$

$G_{B:A:A:A}=G_{A:B:A:A}=G_{A:A:B:A}=G_{A:A:A:B}$

$L_{A,B:*:*:*}=L_{*:A,B:*:*}=L_{*:*:A,B:*}=L_{*:*:*:A,B}$

The asterisk * means that the interaction parameter is independent of the occupation of that sublattice. For the disordered phase to be completely disordered, i.e. that all site fractions are equal on all four sublattices, all constraints must be correct.

For ordered BCC phases, the situation is a bit more complicated, as the four sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase, with A located on two sublattice sites and B on the other two, the end-member described by $G_{A:A:B:B}$ has four nearest neighbour bonds between A and B atoms, whereas the end-member described by $G_{A:B:A:B}$ has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds. Many parameters thus have a relation:

$G_{A:B:B:B}=G_{B:A:B:B}=G_{B:B:A:B}=G_{B:B:B:A}$

$G_{B:A:A:A}=G_{A:B:A:A}=G_{A:A:B:A}=G_{A:A:A:B}$

$G_{A:A:B:B}=G_{B:B:A:A}$

$G_{A:B:A:B}=G_{A:B:B:A}=G_{B:A:A:B}=G_{B:A:B:A}$

$L_{A,B:*:*:*}=L_{*:A,B:*:*}=L_{*:*:A,B:*}=L_{*:*:*:A,B}$

The $G_{A:B:B:B}$ term represents $D0_3$, $G_{A:A:B:B}$ B2 and the $G_{A:B:A:B}$ B32 ordering. There are also two kinds of reciprocal interaction parameters:

$L_{A,B:A,B:*:*;0...9}$

$L_{A,B:*:A,B:*;0...9}$

Kusoffsky et al. (2001) have shown the influence of different parameters available in the 4SL model applied to fcc ordering. The possibility to use the 4SL model to BCC ordering has been studied by Sundman et al. (2009) in the Al-Fe system.

2SL Model for FCC, HCP and BCC

The reason for using a 2SL model instead of a 4SL model is that the calculations are faster, but on the other hand it can only model one kind of ordered phase(s). For instance, it is not possible to model FCC with both $L1_0$ and $L2_1$, or BCC with $D0_3$ and B2, etc.

In order to get the fully disordered phase to form, constraints are needed as for the 4SL model. For the symmetric phases, e.g. B2 and $L1_0$, the relation between parameters are:

$G_{A:B}=G_{B:A}$

$L_{A,B:*}=L_{*:A,B}$

For a 2SL asymmetric model including, but not limited to, $L1_2$, more constraints are needed. This model has many complicated relations between the parameters. The relation between the parameters for the 2SL $L1_2$ model can be derived from a 4SL model. The conversion from 4SL model parameters to 2SL parameters for $L1_2$ can be found in Dupin et al. (2001) and for $L1_0$ in Yuan et al. (2012). Higher-order systems with an $L1_2$ phase modelled with two sublattices require a lot of ternary and some quaternary interaction parameters in order to make the disordered state stable. These parameters have been derived by e.g. Dupin (1995), also found in Kusoffsky et al. (2001).

Many publications exist on how to model order/disorder transformations using a two-sublattice model, see e.g. Dupin, Ansara (1999), De Keyzer et al. (2009).

Magnetic Ordering

The magnetic contribution to the Gibbs energy is given by a model proposed by Inden (1975) and adapted by Hillert and Jarl (1978), and is described by:

```
G=RTln(b+1)f(t)
```

where $t=T/T_C$.

The values of the Curie temperature, T_C, and Bohr magneton number, b, at a certain composition are then used in an optimization procedure to calculate the contribution to Gibbs energy due to magnetic ordering. Curie temperature and Bohr magneton number are given in the command *ENTER_PARAMETER* on page 99 for phases that undergo a magnetic transition:

```
AMEND_PHASE_DESCRIPTION BCC_A2 MAGNETIC -1.0 0.4

ENTER_PARAMETER TC(BCC_A2,FE:VA;0) 298.15 +V1; 6000 N

ENTER_PARAMETER BMAGN(BCC_A2,FE:VA;0) 298.15 +V2; 6000 N
```

The arguments -1 and 0.4 specify the values of parameters in the magnetic model: -1 is the antiferromagnetic factor and 0.4 is the structure factor. Usually the antiferromagnetic factor =-1 for bcc and =-3 for fcc (and other non-bcc phases). The structure factor corresponds to the short range order fraction of the enthalpy. This factor is 0.4 for bcc and 0.28 for non-bcc phases.

Molar Volumes and High Pressure

Including volumes in a thermodynamic database enable calculations of volume changes, volume fraction, lattice mismatch in cubic structures and phase diagrams at increased pressure. Pressure independent volumes can be used up to about 1 GPa. At pressures above 1 GPa the pressure dependence of the volumes must be included by using a proper equation of state (EOS). An EOS has been developed by Lu et al. (2005), based on the EOS from Jacobs and Oonk (2000). Four parameters are used in the implementation of the model in Thermo-Calc:

- `V0`: Volume at 1 bar and at reference temperature T_0
- `VA`: Integrated thermal expansivity
- `VK`: Isothermal compressibility at 1 bar
- `VC`: Parameter to fit high pressure data

All parameters can be composition dependent in the same way as all other model parameters in Thermo-Calc. Experimental information about the temperature, pressure and composition dependence of the volume can be assessed using these model parameters. To evaluate V0, VA and VK experimental data at 1 bar only are needed.

Example

Examples on modelling molar volume in a setup-file:

```
ENTER_PARAMETER V0(BCC_A2,FE:VA;0) 298.15 +V1; 6000 N

ENTER_PARAMETER VA(BCC_A2,FE:VA;0) 298.15 +V2*T+V3*T**2; 6000 N

ENTER_PARAMETER VC(BCC_A2,FE:VA;0) 298.15 +V4+V5*T; 6000 N

ENTER_PARAMETER VK(BCC_A2,FE:VA;0) 298.15 +V6+V7*T; 6000 N

ENTER_PARAMETER V0(FCC_A1,CR,FE:VA;0) 298.15 +V8; 6000 N

ENTER_PARAMETER VA(FCC_A1,CR,FE:VA;0) 298.15 +V9*(T-298.15); 6000 N
```

Excess Models

Unless specifically amended, the excess Gibbs energy terms are modelled by the Redlich-Kister-Muggianu Model. Other excess models for the Gibbs energy are also implemented in Thermo-Calc, such as e.g. Kohler and Toop-Kohler extrapolation models.

Thermo-Calc is not restricted to binary interaction parameters. Ternary, quaternary and higher-order interaction parameters can also be used if there is enough information to evaluate these from experimental data. The ternary interaction parameters are identified by the degrees of the so-called ternary L parameter (i.e. 0, 1 and 2) in the command *ENTER_PARAMETER* on page 99. If the parameter is composition-independent, you only need a single interaction parameter with a degree of zero, i.e. only the ^{0}L term. If there is a ternary composition-dependent interaction parameter, you must enter all three parameters (0,1 and 2). If such a ternary interaction parameter should be zero, then assign it a function which is zero. If the three interaction parameters have the same value, then that is identical to having a composition-independent ternary parameter.

Example

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N

ENTER_PARAMETER L(LIQUID,A,B,C;1) 298.15 +1000; 6000 N

ENTER_PARAMETER L(LIQUID,A,B,C;2) 298.15 +1000; 6000 N
```

is identical to

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

This also means that

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N

ENTER_PARAMETER L(LIQUID,A,B,C;1) 298.15 +ZERO#; 6000 N

ENTER_PARAMETER L(LIQUID,A,B,C;2) 298.15 +ZERO#; 6000 N
```

is NOT identical to

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

Graphical Mode Examples Guide

Version 2016b

Thermo-Calc Software

About the Graphical Mode Examples

These examples are for Thermo-Calc in Graphical Mode. There is a separate set of examples for Thermo-Calc Console Mode.

The Graphical Mode examples are stored without calculated results. In Thermo-Calc, open the example file and select the project icon at the top of the **Project** window. Then right-click and select **Perform now**.

> ⓘ Precipitation Module (TC-PRISMA) examples are included in this folder.

You can open the examples from your computer or download from the website.

Installed Examples

The PDF and example files are also included with your installation in a folder location based on the operating system.

> On Windows, once Thermo-Calc is installed, you can also locate the Examples and Materials folders, plus all the Manuals using the shortcuts located in the Start menu. Go to **Start →** **All Programs** or **All Apps → Thermo-Calc** and click **Examples**, **Manuals**, or **Materials** as required to open the applicable folder.

In the table, <*user*> stands for the username and <*version*> for the version of Thermo-Calc, for example 2016b.

OS	User type	Default directory
Windows	Normal user	Users\\<*user*>\Thermo-Calc\\<*version*> Users\\<*user*>\Documents\Thermo- Calc\\<*version*> My documents
	Administrator	Program Files\Thermo-Calc\\<*version*> Users\Public\Documents\Thermo- Calc\\<*version*> Public documents
Mac	Administrator (user name and password required)	Examples and manuals in /Users/Shared/Thermo-Calc/<*version*> To go to this folder, in Finder, from the **Go** main menu select **Go to folder**. Enter the above file path and click **Go**.

OS	User type	Default directory
Linux	Non root user	home/*<user>*/Thermo-Calc/*<version>*
	Root user	usr/local/Thermo-Calc/*<version>*

Download from the Website

You can also download the PDF and the example files from the website

1. Go to http://www.thermocalc.com/.
2. From the menu, select **Support →Documentation**.
3. Click **Examples** to expand the list.
4. To the right of the example files you want to download, click **Read More**.
5. Click the links to either open a PDF in a browser or to download zipped files containing the examples.

Examples of Thermo-Calc Activities

Example 1: Calculating a Single-Point Equilibrium

This example shows the result from a single-point equilibrium calculation in the Fe-C system. The number of equilibrium conditions is C+2 where C is the number of components, meaning that four conditions are needed in this example:

- **Temperature** is 1000 K
- **Pressure** is 101325 Pa
- **System size** is 1 mole
- **Mass percent carbon** is 0.1%

The displayed results of the calculation show that the BCC_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.

File Name	Activity Example
Ex_01_Single-point_equilibrium	Equilibrium Calculator

Example 2: Stepping in Temperature in the Fe-C System

This example shows how the fractions of stable phases vary for an Fe-0.1 mass-% C alloy when the temperature is varied between 500 and 2000 K. To allow temperature to vary, the corresponding **Axis Definition** check box is selected. In this example, results are displayed graphically using a **Plot Renderer** activity. To get text results a **Table Renderer** activity is used instead.

File Name	Activity Examples
Ex_02_Step_in_temperature_in_Fe-C	Equilibrium Calculator, Plot Renderer and a Table Renderer

Example 3: Fe-C Phase Diagrams

This example shows the stable Fe-C phase diagram (stable meaning that the graphite phase is entered in the calculation). The same diagram is calculated using a:

- **Binary Calculator** activity and a
- **System Definer** and an **Equilibrium Calculator** activity. In both cases, a **Plot Renderer** activity is used to display results. The purpose of the **Binary Calculator** is to simplify common calculations for binary systems. In the **Equilibrium Calculator** two axes are defined: *Mass percent C* and *Temperature*. An axis variable must also be an equilibrium condition.

File Name	Activity Examples
Ex_03_Fe-C_phase_diagram	Binary Calculator, System Definer and Equilibrium Calculator

Example 4: Ternary Phase Diagram in the Fe-Cr-C System at 1000 K

This example shows a ternary phase diagram in the Fe-Cr-C system at 1000 K. Similar to Example 3, the same diagram is calculated using:

- a **Ternary Calculator** activity and
- a **System Definer** and an **Equilibrium Calculator** activity. To toggle between a tri-angular and a rectangular diagram, press the **Show Triangular** button. To toggle the X and Y axis variables, press the **Switch Axes** button.

File Name	Activity Examples
Ex_04_Fe-Cr-C_ternary_phase_diagram	Ternary Calculator, System Definer and Equilibrium Calculator

Example 5: Stable and the Metastable Fe-C Phase Diagrams

This example shows how to overlay results from two calculations in the same plot. In *Equilibrium Calculator 1* the stable phase diagram is calculated and in *Equilibrium Calculator 2* the metastable. The

Plot Renderer activity is first created as a successor to Equilibrium Calculator 1. Then right-click the Plot Renderer node and select **Add predecessor** and the results from both equilibrium calculators are in the same plot. The metastable diagram is obtained by deselecting the graphite phase in the System Definer under the **Phases and phase constitution** tab.

File Name	Activity Example
Ex_05_Fe-C_stable_and_metastable_phase_diagram	Equilibrium Calculator

Example 6: Serially Coupled Equilibrium Calculators

This example shows how to use serially coupled Equilibrium Calculators for more complex equilibrium conditions. Sometimes there are multiple possible solutions for a given set of equilibrium conditions. In other cases the equilibrium calculation does not converge. You can then aid the final calculation by, in effect, telling the software where it should start the search for the equilibrium. Here are examples of two such cases.

- In the first example, the final objective is to calculate the equilibrium at 850◦C where the mole fractions of the FCC A1 and BCC A2 phases are 0.5 each for an Fe-Cr-C steel with 10% chromium. In Equilibrium Calculator 1 a simple set of equilibrium conditions (temperature, pressure, system size and composition) are used to find a carbon content where only the FCC A1 and BCC A2 phases are stable. The results from this preliminary calculation are displayed in Table Renderer 1.
- In Equilibrium Calculator 2 the carbon content equilibrium condition is replaced by the condition that the numbers of moles of the BCC A2 phase should be 0.5. The final result is displayed in Table Renderer 2. In this case, the final objective is to calculate the solidus temperature of an Fe-Cr-C steel with 10% Cr and 0.01% C.
- In Equilibrium Calculator 3 the state at 2000 K is calculated and the result is displayed in Table Renderer 3.
- In Equilibrium Calculator 4 the temperature equilibrium condition is replaced by the condition *Fix phase / liquid / 0.0*, meaning that liquid should be stable in an amount of zero moles, i.e. the solidus temperature. The final result is displayed in Table Renderer 4.

File Name	Activity Example
Ex_06_Serial_equilibrium_calculators	Equilibrium Calculator

Example 7: User-Defined Functions

This basic example shows the use of user-defined functions. A series of equilibria for an Fe-Cr-C alloy are calculated by varying temperature between 500 and 3000 K. In the configuration window of the **Equilibrium Calculator** under the **Functions** tab, two identically meaning functions are defined, *fraction solid* and *f solid*, the values of which are plotted against temperature in the Plot Renderers. Functions can be entered in terms of *QuantitiesQ1*, *Q2*, *Q3* etc., or, for using the Thermo-Calc syntax.

File Name	Activity Example
Ex_07_User_defined_functions	Equilibrium Calculator

Example 8: Scheil and Equilibrium Solidification

This example shows a comparison for an Al-Si alloy solidified under full local equilibrium and under the Scheil assumptions, i.e. zero diffusion in the solidified material and infinitely fast diffusion in the liquid. There are three Plot Renderers created: Scheil solidification, equilibrium solidification and the third Plot Renderer includes both in the same plot.

File Name	Activity Example
Ex_08_Scheil_and_equilibrium_solidification	Scheil Calculator

Example 9: Carbide Driving Force Heat Maps

This is an example of using *property grid* calculations to plot the driving force for a carbide as a function of two composition variables. With the property grid calculation type, a 2D grid is generated from the two calculation axes. After the calculation is done, an equilibrium is calculated in each grid point. A Plot Renderer connected to a property grid calculator plots the *z*-axis property for each equilibrium as a function of the two calculation axes. The final plot can be either a heat map or a contour plot.

File Name	Activity Example
Ex_09_Heat_map_of_carbide_driving_force	Plot Renderer

Example 10: Phase Transition

The example uses the Property Model Calculator to predict the transition temperature to the unwanted brittle Sigma phase. The example shows how the temperature is influenced by changes to a steel alloy’s composition using the uncertainty calculation type and how to create either a histogram or probability plot.

File Name	Activity Example
Ex_10_Phase_Transition	Property Model Calculator

Example 11: Coarsening and Interfacial Energy

The example uses the Property Model Calculator and both thermodynamic and kinetic demonstration steel databases. Using a grid calculation type it produces three plots: a heat map, a contour plot and a cross plot with contour (where both the interfacial energy and coarsening rate is shown).

File Name	**Activity Example**
Ex_11_Coarsening_and_Interfacial_energy	Property Model Calculator

Example 12: Driving Force and Interfacial Energy

The example uses the Property Model Calculator and a thermodynamic demonstration steel database. Using a grid calculation type it produces a contour plot comparing the driving force and interfacial energy.

File Name	**Activity Example**
Ex_12_Driving_force_and_Interfacial_energy	Property Model Calculator

Precipitation Calculator Examples

Examples 13 and 16 are available to all users. The other examples require a Precipitation Module (TC-PRISMA) license to calculate and plot results.

All examples use demonstration database packages included with your installation.

Example 13: Isothermal Precipitation of Al_3Sc

This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase. The simulation results can be compared with experimental data collected from Marquis and Seidman[1] and Novotny and Ardell[2].

Details and Plot Example

System	
Database package	Demo: Aluminum-based alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Matrix phase	FCC_A1

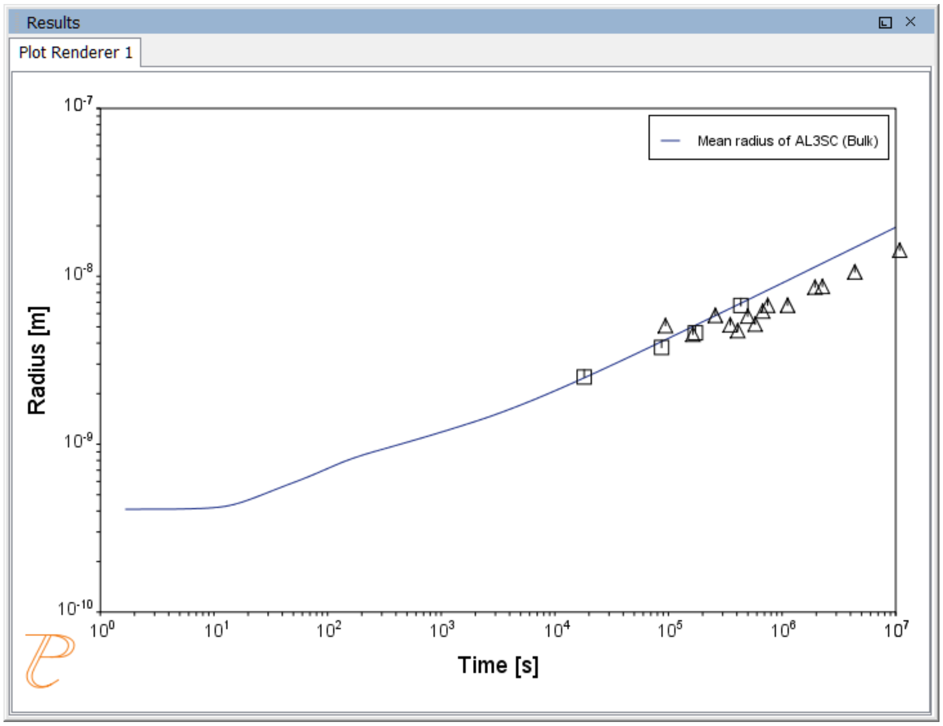
---

[1] E. Marquis, D.. Seidman, Nanoscale structural evolution of Al3Sc precipitates in Al(Sc) alloys, Acta Mater. 49 (2001) 1909–1919.

[2] G.M. Novotny, A.J. Ardell, Precipitation of Al3Sc in binary Al–Sc alloys, Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process. 318 (2001) 144–154.

Precipitate phases	AL3SC
Conditions	
Composition	Al-0.18Sc Mole percent
Temperature	350° C
Simulation time	1.0E7 seconds
Nucleation sites	Bulk
Precipitate Phase Data Parameters	
Interfacial energy	Calculated
Other	
Calculation type	Isothermal
File name	Ex_13_Precipitation_Al-Sc_AL3SC.tcu

Plot Results



Example 14: Stable and Metastable Carbides - Isothermal

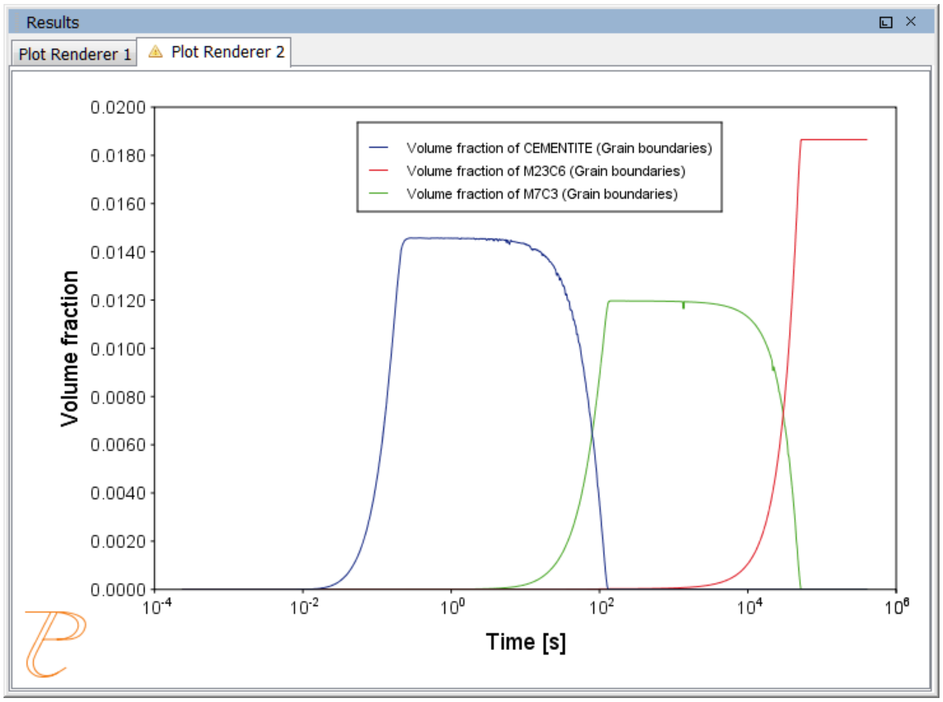
This example simulates the kinetics of precipitation of both stable and metastable carbides from ferrite phase. It demonstrates that metastable carbides (cementite, M7C3) may first emerge and then disappear and the stable phase (M23C6) prevails.

Details and Plot Example

This example uses the Equilibrium Calculator and a property diagram to determine how the phases change with temperature. We are interested in the carbide precipitation at 1053K where only the carbide M23C6 is stable according to the equilibrium calculation. The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6 and M7C3) where cementite and M7C3 are metastable phases.

System	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)
Elements	Fe, C, Cr
Matrix phase	BCC_A2
Precipitate phases	Cementite, M23C6 and M7C3
Conditions	
Composition	Fe-0.1C-12Cr Mass percent
Temperature	1053 K
Simulation time	400 000 seconds
Nucleation sites	Grain boundaries
Matrix Phase Data Parameters	
Grain radius	1.0E-4 m
Precipitate Phase Data Parameters	
Interfacial energy	Cementite 0.174 J/m^2, M23C6 0.26 J/m^2, M7C3 0.3 J/m^2
Other	
Calculation type	Isothermal
File name	Ex_14_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6

Plot Results



Example 15: Stable and Metastable Carbides - TTT Diagram

In this example, the kinetics of precipitation of both stable and metastable carbides is calculated from the ferrite phase. It demonstrates that metastable carbides may first emerge and then disappear and the stable phase prevails.

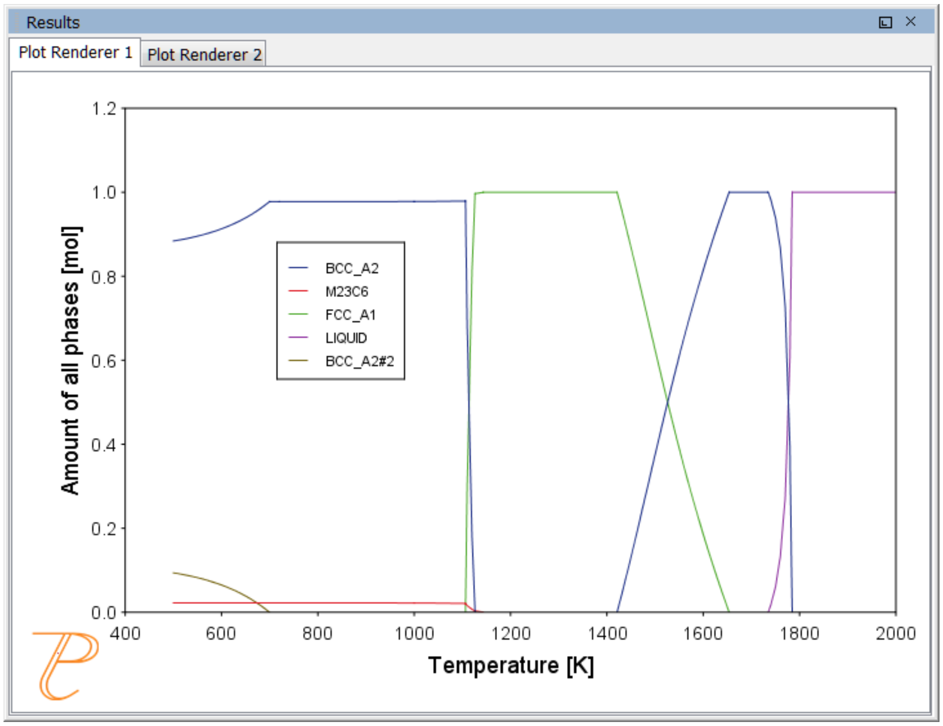
Details and Plot Example

This example uses the Equilibrium Calculator and a property diagram to determine how the phases change with temperature. Using this result, the Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

System	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)
Elements	Fe, C, Cr
Matrix phase	BCC_A2

Precipitate phases	Cementite, M23C6 and M7C3
Conditions	
Composition	Fe-0.1C-12Cr Mass percent
Temperature	500° to 800° C with 25°C steps
Max. simulation time	1.0E8 seconds
Nucleation sites	Grain boundaries
Matrix Phase Data Parameters	
Grain radius	1.0E-4 m
Precipitate Phase Data Parameters	
Interfacial energy	Cementite 0.174 J/m^2, M23C6 0.26 J/m^2, M7C3 0.3 J/m^2
Other	
Calculation type	TTT diagram
Stop criterium	Volume fraction of phase is set to 0.0001
File name	Ex_15_Precipitation_Fe-C-Cr_TTT_Cementite-M7C3-M23C6

Plot Results



Example 16: Precipitation of Iron Carbon Cementite

Simulate the kinetics of precipitation of carbides from a BCC Fe solution phase. This example is based on Wert (1949)[1].

Details and Plot Example

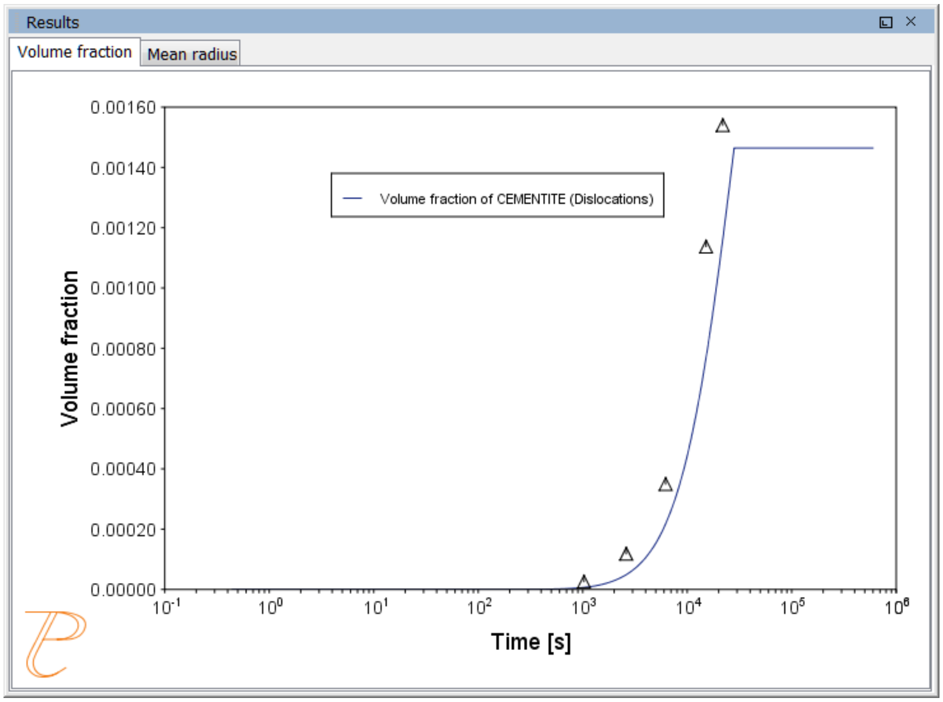
This example uses two Experimental File Reader activities with the Precipitation Calculator and an isothermal calculation, to plot the volume fraction of the cementite phase.

System	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)
Elements	Fe, C
Matrix phase	BCC_A2
Precipitate phase	Cementite
Conditions	
Composition	Fe-0.016C mass percent
Temperature	102° C
Simulation time	600 000 seconds
Nucleation sites	Dislocations
Matrix Phase Data Parameters	
Grain aspect ratio	1.0
Precipitate Phase Parameters	
Interfacial energy	0.24 J/m^2
Dislocation density	1.5e11m^{-3}
Other	
Calculation type	Isothermal
Growth rate model	Advanced (on the Options tab)
File name	Ex_16_Precipitation_Fe-C_Cemetite

---

[1] Wert, C. A. (1949). Precipitation from Solid Solutions of C and N in α-Iron. Journal of Applied Physics, 20(10), 943.

Volume Fraction



Example 17: Precipitation of γ′ in Ni Superalloys - Isothermal

This example simulates the kinetics of precipitation of γ′ phase from γ phase. The simulation results can be compared with experimental data collected from Sudbrack et al.[1].

Details and Plot Examples

This example uses three Experimental File Reader activities with the Precipitation Calculator. It does an isothermal calculation to plot the volume fraction, mean radius and number density of the cementite phase.

DIS_FCC_A1 needs to be selected on the System Definer. Search the online help for **About Ordered Phases** in the *Precipitation Module (TC-PRISMA) User Guide* for details.

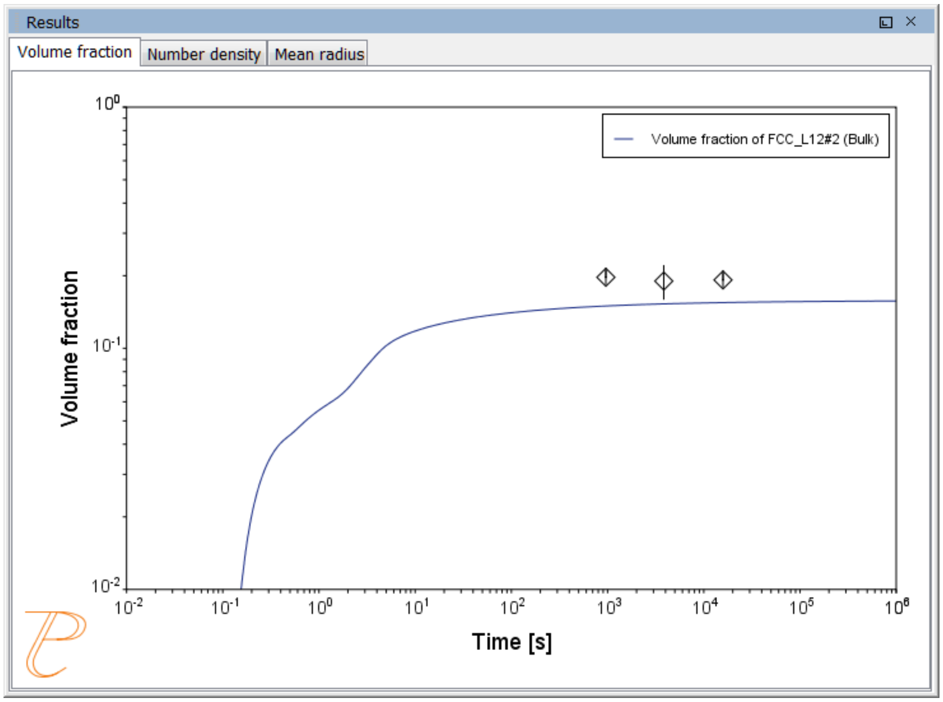
System	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al Cr

---

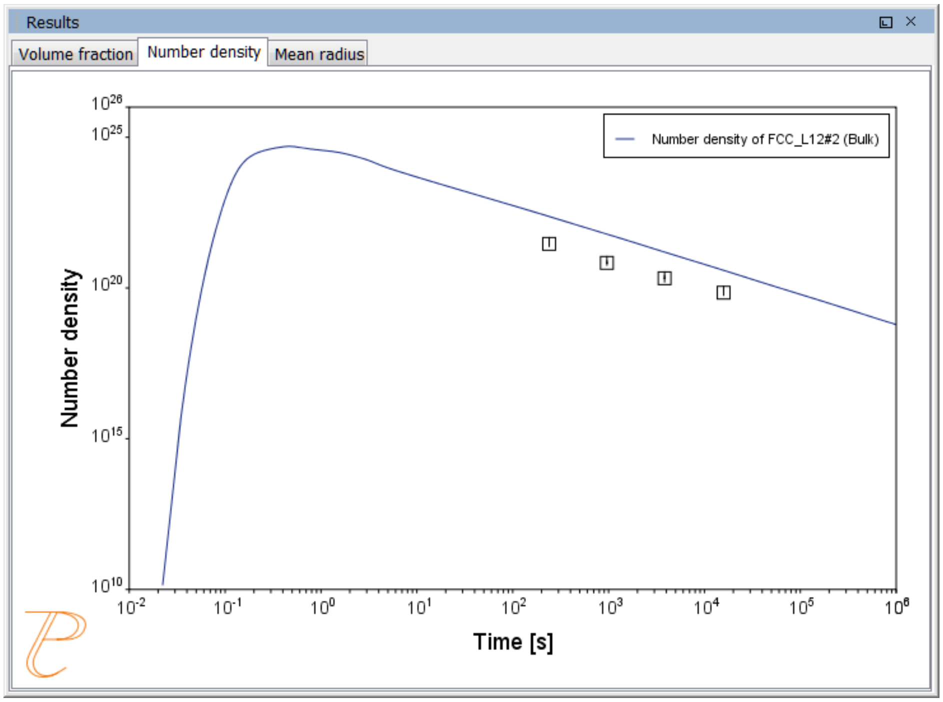
[1] C.K. Sudbrack, T.D. Ziebell, R.D. Noebe, D.N. Seidman, Effects of a tungsten addition on the morphological evolution, spatial correlations and temporal evolution of a model Ni–Al–Cr superalloy, Acta Mater. 56 (2008) 448–463.

Matrix phase	DIS-FCC_A1 (see note above about how to select this phase)
Precipitate phase	FCC_L12#2
Conditions	
Composition	Ni-9.8Al-8.3Cr Mole percent
Temperature	800° C
Simulation time	1 000 000 seconds
Nucleation sites	Bulk
Precipitate Phase Data Parameters	
Interfacial energy	0.023 J/m^2
Other	
Calculation type	Isothermal
File name	Ex_17_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime

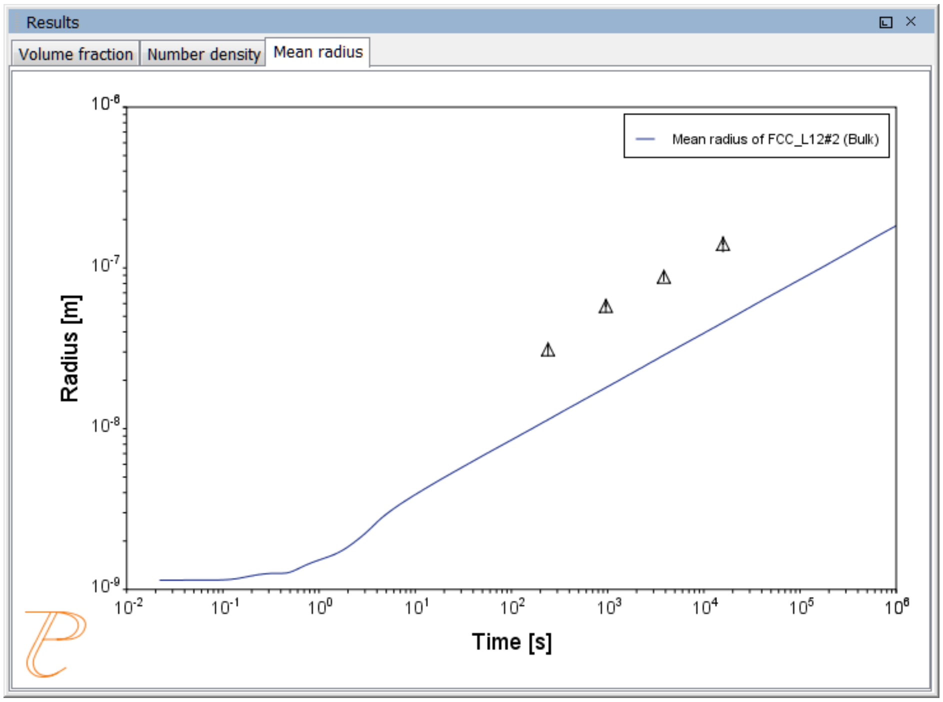
Volume Fraction



Number Density



Mean Radius



Example 18: Precipitation of γ' in Ni Superalloys - Non-isothermal

This example simulates the kinetics of precipitation of γ' phase from γ phase in Ni-8Al-8Cr and Ni-10Al-10Cr at.% alloys during continuous cooling. The simulation results can be compared with experimental results from Rojhirunsakool et al.[1] .

Details and Plot Examples

In these examples the Separate multimodal PSD check box is selected on the Plot Render to plot the mean radius and size distributions of the two compositions.

Plotting the size distribution from the final simulation time of 1470 seconds, you can see there are several peaks, although these are not completely separated. Use the 'Separate multimodal PSD' check box on the Plot Renderer to separate the peaks. Then adjust the Valley depth ratio setting to 0.05 to separate into two peaks as shown in the Ni-10Al-10Cr plot example. You can experiment with this setting to see how the size distribution evolves with time, for example, try entering several values as plot times '400 600 1470'.

DIS_FCC_A1 needs to be selected on the System Definer. Search the online help for **About Ordered Phases** in the *Precipitation Module (TC-PRISMA) User Guide* for details.

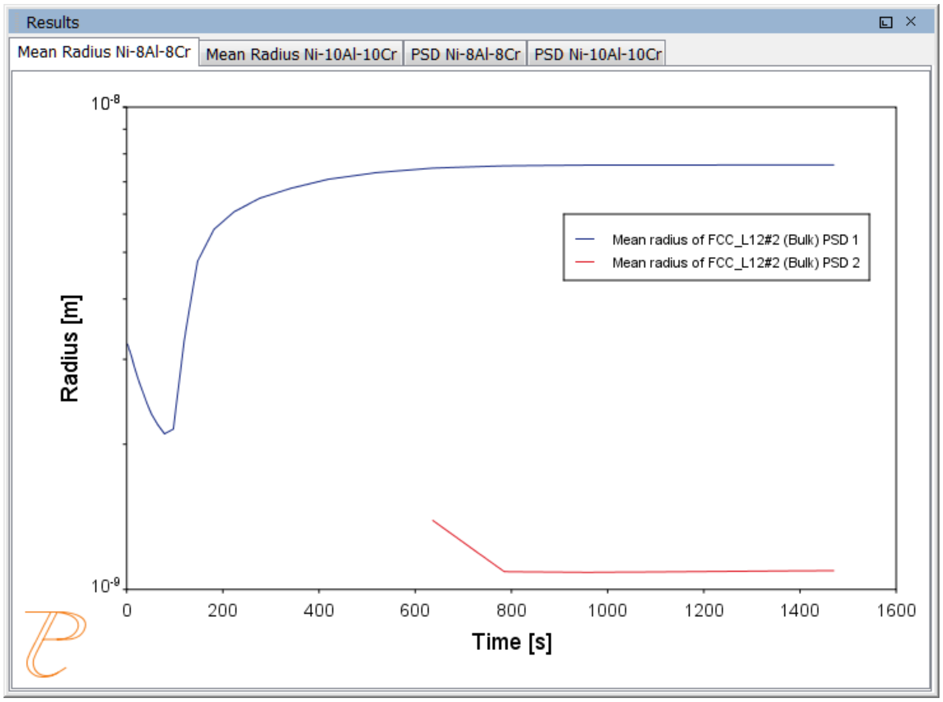
System	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Matrix phase	DIS_FCC_A1 (see note above about how to select this phase)
Precipitate phase	FCC_L12#2
Conditions	
Composition (Ni-8Al-8Cr)	Ni-8Al-8Cr Mole percent
Composition (Ni-10Al-10Cr)	Ni-10Al-10Cr Mole percent
Temperature	0.23 K/s cooling rate
Simulation time	1470 s (Ni-8Al-8Cr), 3300 s (Ni-10Al-10Cr)

---

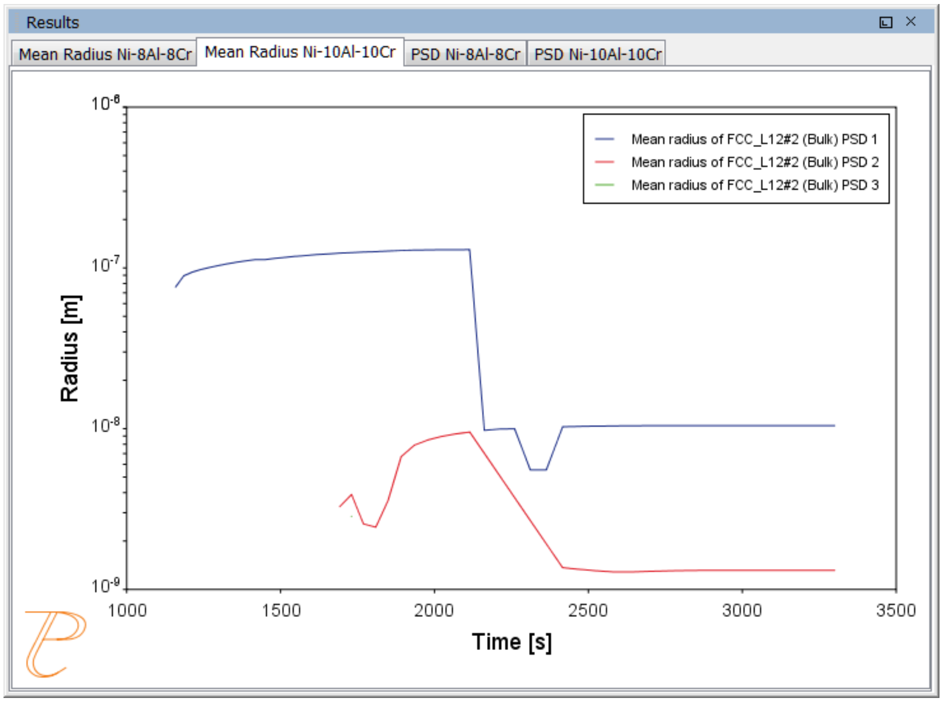
[1] T. Rojhirunsakool, S. Meher, J.Y. Hwang, S. Nag, J. Tiley, R. Banerjee, Influence of composition on monomodal versus multimodal γ' precipitation in Ni–Al–Cr alloys, J. Mater. Sci. 48 (2013) 825–831.

Nucleation sites	Bulk
Matrix Phase Data Parameters	
Mobility enhancement prefactor	5.0
Precipitate Phase Data Parameters	
Interfacial energy	0.023 J/m^2
Other	
Calculation type	Non-isothermal
Separate multimodal PSD for 8Al-8Cr	On the Plot Renderer, the Valley depth ratio is set to 0.05 for both plots. The number of points is increased to 200 for an average radius plot.
Separate multimodal PSD for 10Al-10Cr	On the Plot Renderer, the Valley depth ratio is set to 0.18 for both plots.
File name	Ex_18_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime

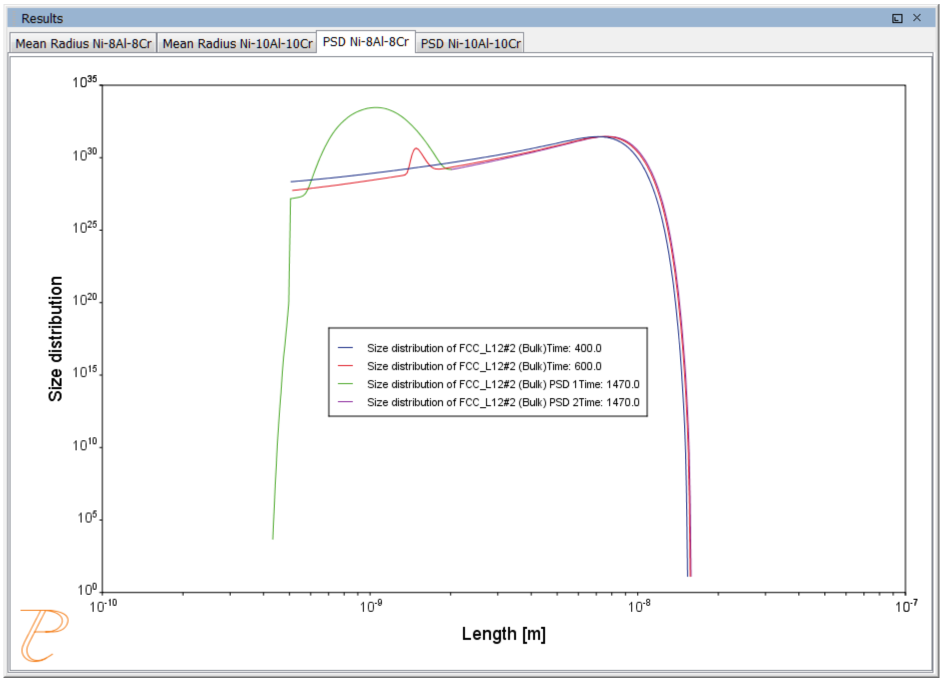
Mean Radius Ni-8Al-8Cr



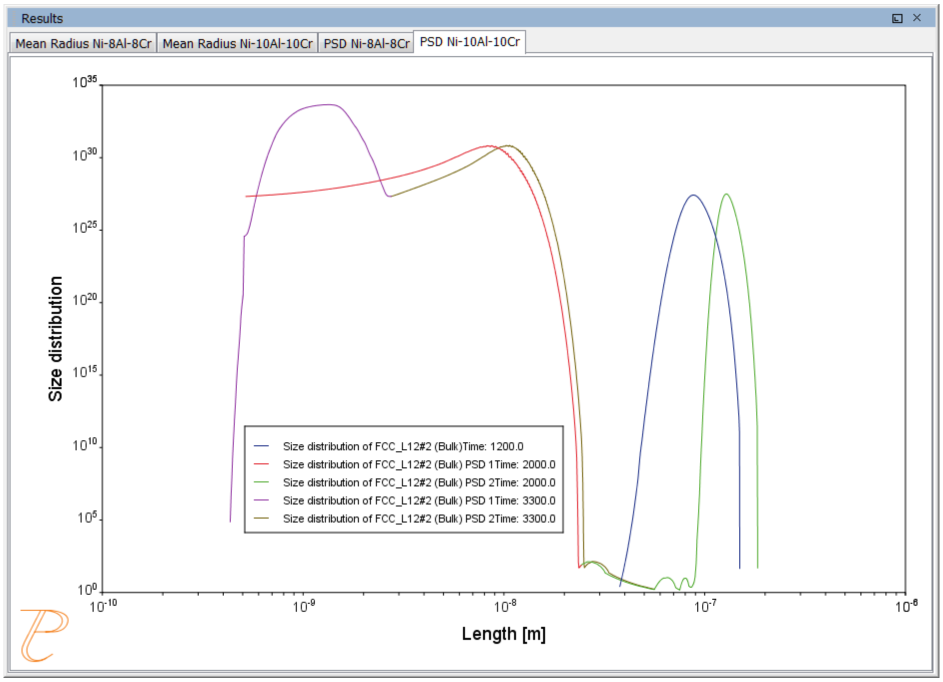
Mean Radius Ni-10Al-10CR



Size Distribution (PSD) Ni-8Al-8Cr

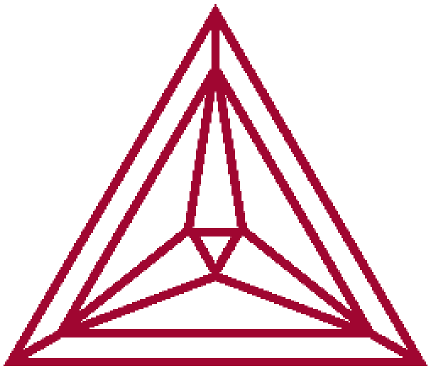


Size Distribution (PSD) Ni-10Al-10Cr



Console Mode Examples Guide

Version 2016b



Thermo-Calc
Software

About the Console Mode Examples Guide

This guide is available as a PDF.

For descriptions of each example, see *Console Mode Example Collection* on page 14.

Installed Examples

The PDF and example files are also included with your installation in a folder location based on the operating system.

On Windows, once Thermo-Calc is installed, you can also locate the Examples and Materials folders, plus all the Manuals using the shortcuts located in the Start menu. Go to **Start →** **All Programs** or **All Apps → Thermo-Calc** and click **Examples**, **Manuals**, or **Materials** as required to open the applicable folder.

In the table, <*user*> stands for the username and <*version*> for the version of Thermo-Calc, for example 2016b.

OS	User type	Default directory
Windows	Normal user	Users\<*user*>\Thermo-Calc\<*version*> Users\<*user*>\Documents\Thermo- Calc\<*version*> My documents
	Administrator	Program Files\Thermo-Calc\<*version*> Users\Public\Documents\Thermo- Calc\<*version*> Public documents
Mac	Administrator (user name and password required)	Examples and manuals in /Users/Shared/Thermo-Calc/<*version*> To go to this folder, in Finder, from the **Go** main menu select **Go to folder**. Enter the above file path and click **Go**.
Linux	Non root user	home/<*user*>/Thermo-Calc/<*version*>
	Root user	usr/local/Thermo-Calc/<*version*>

Download from the Website

You can also download the PDF and the example files from the website

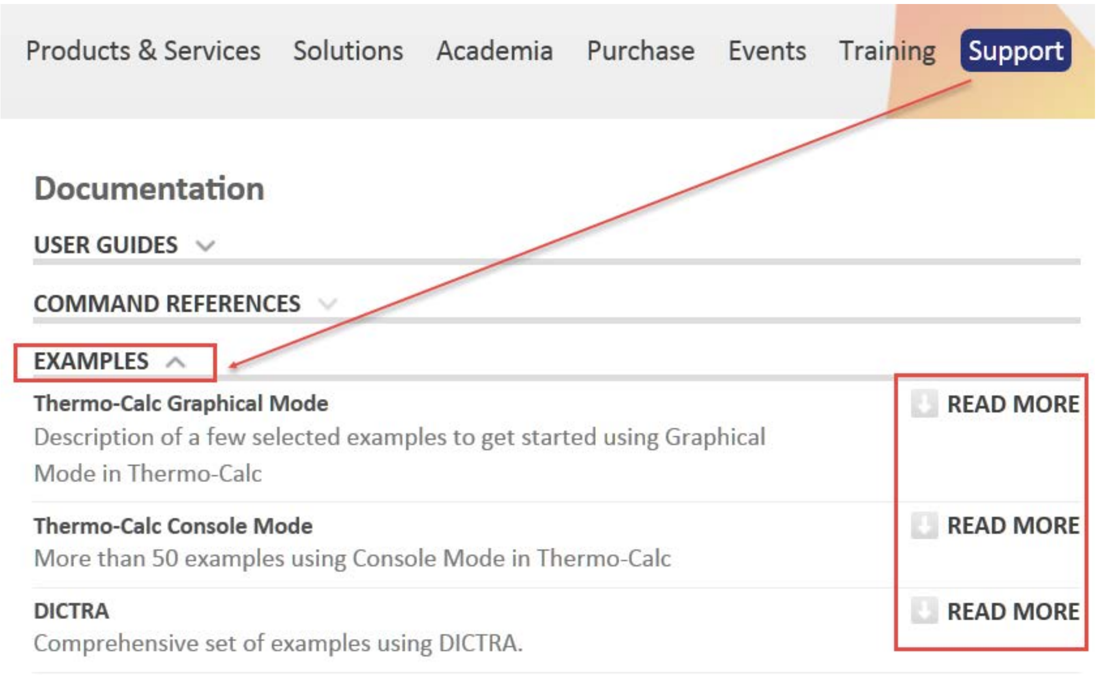
1. Go to http://www.thermocalc.com/.

2. From the menu, select **Support →Documentation**.

3. Click **Examples** to expand the list.

4. To the right of the example files you want to download, click **Read More**.

5. Click the links to either open a PDF in a browser or to download zipped files containing the examples.



Documentation

Thermo-Calc Graphical Mode
Description of a few selected examples to get started using Graphical Mode in Thermo-Calc

Thermo-Calc Console Mode
More than 50 examples using Console Mode in Thermo-Calc

DICTRA
Comprehensive set of examples using DICTRA.

Thermo-Calc Software

Console Mode Examples Guide

Thermo-Calc Version 2016a

Stockholm, Sweden

tcex01

Calculation of the Fe-C binary phase diagram.

tcex02

Plotting of thermodynamic functions in unary, binary and ternary systems and working with partial derivatives and partial quantities

tcex03

Calculation of an isothermal section using TERNARY module

tcex04

Calculation of the miscibility gap in Fe-Cr

tcex05

Calculation of a vertical section in the Al-Cu-Si system Calculation of a vertical section from Al to 10% cu2Si

tcex06

Calculation of an isopleth in low alloyed Fe-Mn-Si-Cr-Ni-C steel. Calculation of a multicomponent phase diagram.

tcex07

Calculation of single equilibria in low alloyed Fe-Mn-Si-Cr-Ni-C steel.

tcex08

Calculation of a property diagram for a high speed steel i.e. phase fraction plots, activity vs temperature etc.

tcex09

Calculation of dew point

tcex10

Preventing clogging of Cr2O3 in a continuous casting process

tcex11

Oxidation of Cu2S with H2O/O2 gas

tcex12

Tabulation of thermodynamic data for reactions

tcex13

Calculation of phase diagram and G curve using the BINARY module

tcex14

Calculation of the variation of the heat and the heat capacity during solidification of an Al-Cu-Si alloy

tcex15

This is an example of a solidification simulation of a Cr-Ni alloy. No back diffusion in the solid, i.e. Scheil-Gulliver model.

tcex16

Calculation of the second order transition line in the Bcc field of the Al-Fe system

tcex17

Calculation of the pseudo-binary system CaO-SiO2 using the ionic database

tcex18

Calculation of the A3 temperature of a steel and the influence of each alloying element on this temperature

tcex19A

Mapping of univariant equilibria with the liquid in Al-Cu-Si Part A: step-by-step calculation

tcex19B

Mapping of univariant equilibria with the liquid in Al-Cu-Si Part B: using TERNARY module

tcex20

Example showing how to calculate an adiabatic decompression using the geochemical database

tcex21

Demonstrates the use of a user-defined database, calculate a ternary isotherm in Fe-Cr-Ni.

tcex22

Calculation of a heat balance. In this case C3H8 is burned in oxygen and the adiabatic flame temperature is calculated.

tcex23

Calculation of T-zero and paraequilibria in a low alloyed steel

tcex24

Simulation of the silicon arc furnace using the REACTOR module

tcex25

Simulation of steel refining

tcex26

Plotting of the partial pressure of gas species along the solubility lines in the As-Ga Phase diagram

tcex27

Example of CVD calculation

tcex28

Example showing calculation of PRE (Pitting Resistance Equivalence) for a duplex stainless steel

tcex29

Calculation of speciation of a gas

tcex30A

Example of Scheil calculation for Al-4Mg-2Si-2Cu Part A: step-by-step calculation

tcex30B

Example of Scheil calculation for Al-4Mg-2Si-2Cu Part B: using SCHEIL module

tcex31

Calculations of CVM and comparisons with sublattices of a fictitious A B system. Also shows how to overlay diagrams from two calculations

tcex32

Calculation of oxide layers on steel and show how to append databases

tcex33

Benchmark calculation for Fe-Cr-C isopleth

tcex34

Calculation of the phase diagram and G curves in the Al-Zn system

tcex35

Example of use of the POTENTIAL module

tcex36a

Assessment. The use of the PARROT module

tcex37

Calculation of an isothermal section, using command-lines

tcex38

Calculation of the Morral "rose"

tcex39

The Calculation of the Reversible Carnot Cycle of Heat Engine

tcex40

POURBAIX module

tcex41

Calculation of a solubility product

tcex42

Paraequilibrium calculation - Formation of Para-pearlite - Isopleth

tcex43

Paraequilibrium calculation - Formation of Para-pearlite - Isothermal

tcex44

Exploring the usage of variables and functions. Proof strength for an austenitic stainless steel at elevated temperatures.

tcex45

3D-Diagram with the gamma volume in the Fe-Cr-C system

tcex46

3D-Diagram with the liquidus surface of the Fe-Cr-C system

tcex47

3D-Diagram A quarternay diagram with the gamma volume in the Fe-Cr-Ni-C system at 1373K

tcex48

Scheil solidification with C back diffusion in solid phases and comparison with simple Scheil and equilibrium calculations.

tcex49

Quasichemical Model via GES

tcex50

Quasichemical Model via TDB

tcex51

Calculation of molar volume, thermal expansivity and density.

tcex52

Changing the excess models for interaction parameters in a solution phase

tcex53

Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine

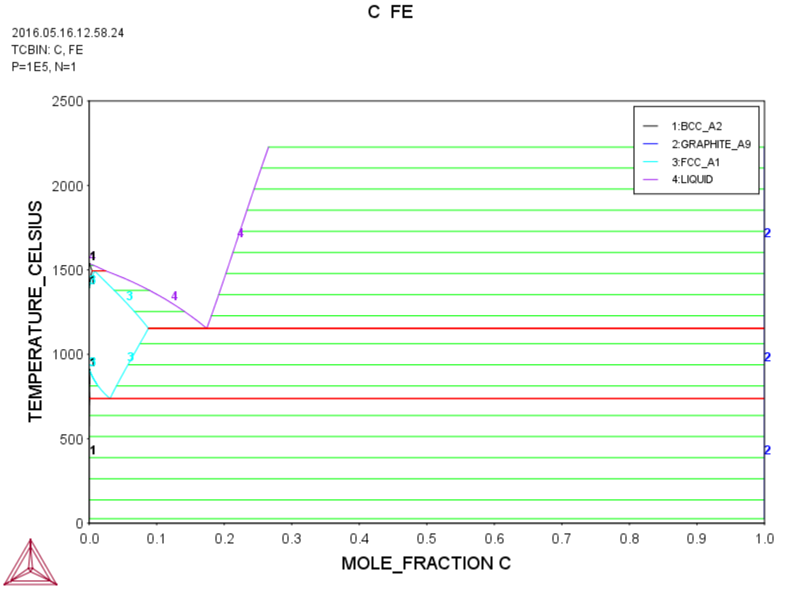
tcex01

```
About Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex01\tcex01.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of the Fe-C binary phase diagram.
SYS: @@
SYS: set-log ex01,,,
SYS:
SYS: @@ The log file is set to get command echo.
SYS: @@ The menu is shown by typing a question mark "?"
SYS: ?
   ... the command in full is HELP
 ABOUT                     HP_CALCULATOR             SET_LOG_FILE
 BACK                      INFORMATION               SET_PLOT_ENVIRONMENT
 CLOSE_FILE                MACRO_FILE_OPEN           SET_TC_OPTIONS
 DISPLAY_LICENSE_INFO      OPEN_FILE                 SET_TERMINAL
 EXIT                      SET_COMMAND_UNITS         STOP_ON_ERROR
 GOTO_MODULE               SET_ECHO
 HELP                      SET_INTERACTIVE_MODE
SYS: @@ When you give a command the program may ask questions.
SYS: @@ You may obtain help for each question by typing a ? .
SYS: @@ If you accept the default answer suggested /within slashes/
SYS: @@ just press "return"
SYS: info
   ... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/: ?

 WHICH SUBJECT

 Specify a subject (or its abbreviation as long as it is unique, e.g.,
 TCC, TC4A, TCW, TC4U, TAB, TDB, TERN, TC-TOOLBOX, THERMO-CALC ENGINE,
 TQ, TCMI, etc.) on which information should be given, from the following
 subjects that are important to the use of the SYS Module:

  PURPOSE (Introducing the THERMO-CALC Software Package)
  COMPUTATIONAL THERMODYNAMICS
  TCC - THERMO-CALC CLASSIC         TCW - THERMO-CALC WINDOWS
  TC4A - THERMO-CALC FOR ACADEMIC   TC4U - THERMO-CALC FOR UNIVERSITY
  MODELS IN THERMO-CALC             MODULES OF THERMO-CALC
  DATABASES IN THERMO-CALC          FUNCTIONALITY OF THERMO-CALC
  STATE VARIABLES                   INTENSIVE VARIABLES
  EXTENSIVE VARIABLES               DERIVED VARIABLES
  UNITS                             BASIC UNITS
  SYSTEM UNITS                      COMPONENT UNITS
  PHASE UNITS                       PHASE-COMPONENT UNITS
  PHASE-SPECIES UNITS               USER-SPECIFIED UNITS
  PHASE DIAGRAMS                    PROPERTY DIAGRAMS
  TDB (DATABASE RETRIEVAL)          GES (GIBBS_ENERGY_SYSTEM)
  POLY (EQUILIBRIUM CALCULATIONS)   POST (POST_PROCESSOR)
  PARROT (ASSESSMENT)               ED_EXP (EDIT_EXPERIEMENT)
  BIN (BINARY_DIAGRAM)              TERN (TERNARY_DIAGRAM)
  POT (POTENTIAL_DIAGRAM)           POURBAIX (POURBAIX_DIAGRAM)
  TAB (TABULATION)                  CHEMICAL EQUATION
  SCHEIL (SCHEIL_SIMULATION)        REACTOR (REACTOR_SIMULATOR)
  SYS (SYSTEM_UTILITY)              FOP (FUNCTION_OPT_PLOT)
  USER INTERFACE OF THERMO-CALC     GUI (GRAPHICAL USER INTERFACE)
  APPLICATIONS OF THERMO-CALC       THERMO-CALC ENGINE
  API - PROGRAMMING INTERFACE       TQ/TCAPI INTERFACES
  TC-TOOLBOX IN MATLAB SOFTWARE     TCMI MATERIALS INTERFACE
  GLOBAL (Global Minimization Technique in the Thermo-Calc software)
  DICTRA (Diffusion-Controlled Transformation Simulation Software)
  HELP   (How to get on-line help in the TCC software)
  NEWS   (Revision History and New Features of the TCC Software)


WHICH SUBJECT /PURPOSE/:
 PURPOSE

              INTRODUCTION to the System Utility Module (SYS)
           *****************************************************

 Thermo-Calc is one of the most powerful and flexible software package
 in the field of Computational Thermodynamics. It has been widely used
 for all kinds of thermochemical calculations of complicated heterogeneous
 phase equilibria and multicomponent phase diagrams. Available for most
 platforms, the Thermo-Calc software provides you with basic thermodynamic
 necessities, such as equilibrium calculations, phase and property diagrams,
 and thermodynamic factors (driving forces) in multicomponent systems.

 Thermo-Calc features a wide spectrum of models, making it possible to
 perform calculations on most complex problems involving thermodynamics.

 Thermo-Calc consists of several basic and advanced modules for equilibrium
 calculations, phase and property diagram calculations, tabulation of
 thermodynamic quantities, database management, assessment of model
 parameters, experimental data manipulations, and post-processing of
 graphical presentations.

 Thermo-Calc facilitates a comprehensive data bank of assessed thermochemical
 data for the phases in various systems, and there are many comprehensive
 databases covering a very wide range of industrial materials and applications.

 Thermo-Calc enables you to establish your own databases through critical
 assessment based on all kinds of experimental information.

 Thermo-Calc utilizes a flexible user interface that is easy to use.
 Additionally, a complete GUI (graphical user interface) version, i.e.,
 TCW (Thermo-Calc Windows), has been developed.
```

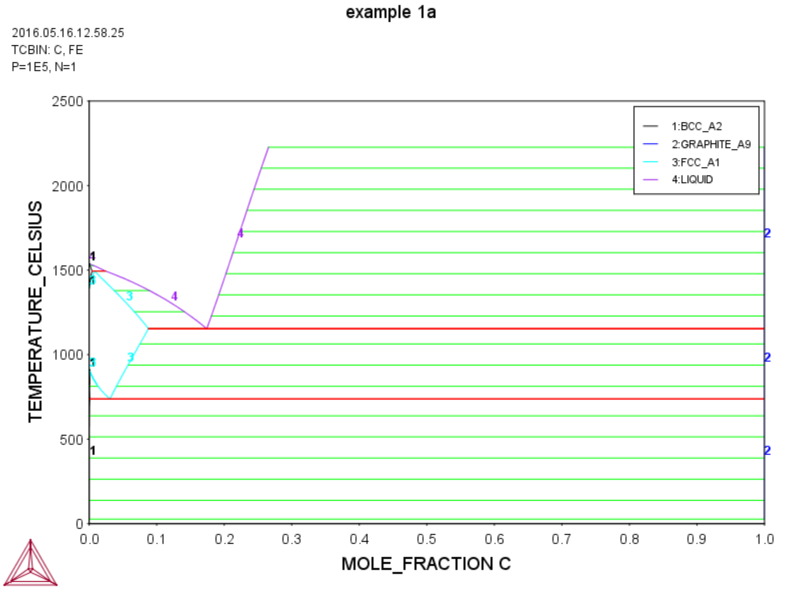
```
 Thermo-Calc presents the standard thermodynamic calculation engine that
 has the fastest and most stable mathematical and thermodynamic solutions.
 Any other software that requires precisely calculated thermochemical
 quantities can make use of the Thermo-Calc Engine through the TQ and
 TCAPI programming interfaces.

 The advantages of Thermo-Calc are its multiple applications. Several
 departments or divisions at the same company, institute or university
 can use the packages for different purposes. Proven application examples
 include industries such as steel plants, aerospace, transportation, and
 manufacturing. With the facilities provided by Thermo-Calc, you can
 optimize your materials processes to produce a higher yield, better
 product at a lower cost.


 The classical versions of both Thermo-Calc and DICTRA software have a
 so-called System Utility Module (under the SYS prompt), which provides
 the primary controls on inter-module communication, MACRO-file creation
 and operation, working and plotting environmental setting, and command
 information searching. They are essential for properly performing ordinary
 calculations, desirably obtaining calculated results, and easily conducting
 various tasks.

 It also facilitates some odd features, such as user interface setting,
 command unit setting, error reporting preference, terminal characteristics
 definition, workspace listing, open or close of a file through a unit,
 interactive calculator, news retrieval, etc. Some of such odd commands
 are used for performance preference of the users, and some are designed
 for debugging of the programmers. Few odd commands are included only for
 some special purposes, which might have been obsolete in later versions.

 The following commands are available in the SYS module:
  SYS:?
   BACK                     HP_CALCULATOR            SET_INTERACTIVE_MODE
   CLOSE_FILE               INFORMATION              SET_LOG_FILE
   EXIT                     MACRO_FILE_OPEN          SET_PLOT_ENVIRONMENT
   GOTO_MODULE              OPEN_FILE                SET_TERMINAL
   HELP                     SET_COMMAND_UNITS        STOP_ON_ERROR
  SYS:

 Notes for versions since TCCR:
  * Five SYS commands have been taken away from the SYS-Module monitor
      (and also eliminated from this chapter in the TCCR User's Guide),
      because they are normally for system debugging purpose only, or
      obsolete now, or totally irrelevant. Such commands include: NEWS,
      LIST_FREE_WORKSPACE, PATCH, SET_ERROR_MESSAGE_UNIT and TRACE.
  * The Section 14.3 (Display of General Information) has been completely
      removed from this chapter since the TCCR User's Guide. However, for
      the purpose of obtaining information about various subjects in
      the SYS module, please use the on-line help feature of the TCCR
      software, i.e., typing the INFORMATON <SUBJECT> command sequence
      in the SYS module, that will follow a display on screen of some
      brief information on a certain subject related to the Thermo-Calc
      software/database/interface package.
  * The FOP Module (FUNC_OPT_PLOT, the simple function optimizer and
      plotting facility; for function/parameter mathematic-fitting and
      plotting) has been completely eliminated from the TCCR software.
      One should instead use the PARROT module to perform critical
      thermodynamic assessments.
  * In the meantime, the SYS command SET_ECHO (that has been blindly
      existing in the TCC and DICTRA software for a very long time)
      is documented in the current edition of this chapter in the
      TCCR User's Guide; see Section 14.2.6 and 14.2.8.

 Revision History of the SYS Module User's Guide:
 =================================================
  Mar 1985  First release
                    (Edited by Bo Sundman)
  Oct 1993  Second revised release
                    (Edited by Bo Sundman)
  Sept 1996 Third revised release
                    (Edited by Mikael Schalin and Bo Sundman)
  Jun 2000  Fourth revised and extended release
                    (Edited by Pingfang Shi)
  Nov 2002  Fifth revised release
                    (Edited by Pingfang Shi)
  Jun 2004  Sixth revised and extended release
                    (Edited by Pingfang Shi)
  Aug 2006  Seven revised and simplified release
                    (Edited by Pingfang Shi)



WHICH SUBJECT:
SYS:Hit RETURN to continue
SYS: @@ For a binary phase diagram calculation we use the binary module
SYS: go
   ... the command in full is GOTO_MODULE
MODULE NAME: ?
 NO SUCH MODULE, USE ANY OF THESE:
 SYSTEM_UTILITIES
 GIBBS_ENERGY_SYSTEM
 TABULATION_REACTION
 POLY_3
 DICTRA_MONITOR
 BINARY_DIAGRAM_EASY
 DATABASE_RETRIEVAL
 DIC_PARROT
 REACTOR_SIMULATOR_3
 PARROT
 POTENTIAL_DIAGRAM
 SCHEIL_SIMULATION
 OLD_SCHEIL_SIM
 POURBAIX_DIAGRAM
 TERNARY_DIAGRAM
MODULE NAME: BIN
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
```

```
 Current database: TC Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: fe
Second element: c
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase-Diagram
   ... the command in full is REJECT
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 C                       FE  DEFINED
 LIQUID:L                IONIC_LIQUID:Y          FCC_A1
 BCC_A2                  A2_BCC                  HCP_A3
 HCP_ZN                  DIAMOND_A4              GRAPHITE_A9
 CBCC_A12                CUB_A13                 B2_FEPD
 C14_LAVES               C15_LAVES               D011_CEMENTITE
 D82_FEZN_GAMMA          L12_FEPD3               AL5FE4
 FE3AS2                  FEZN4                   FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 BCC_A2  RESTORED
 D011_CEMENTITE  RESTORED
 GRAPHITE_A9  RESTORED
 DIAMOND_A4  RESTORED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'P Gustafson, Scan J Metall 14(1985) p 259-267; C-Fe'
 -OK-
   ... the command in full is SET_AXIS_VARIABLE
 The condition X(FE)=.1234  created
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=1319.08  created
   ... the command in full is SET_REFERENCE_STATE
   ... the command in full is SET_REFERENCE_STATE
   ... the command in full is SAVE_WORKSPACES
   ... the command in full is SET_CONDITION
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
 Start points provided by database
   ... the command in full is SAVE_WORKSPACES
 Version S mapping is selected

 Organizing start points

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   9.944E-01  1.100E+03
     BCC_A2
  ** FCC_A1
 Calculated.                       5  equilibria

 Phase region boundary   2 at:   9.838E-01  1.011E+03
     BCC_A2
  ** FCC_A1
  ** GRAPHITE_A9

 Phase region boundary   3 at:   4.996E-01  1.011E+03
     BCC_A2
  ** GRAPHITE_A9
 Calculated..                      30  equilibria
 Terminating at axis limit.

 Phase region boundary   4 at:   4.845E-01  1.011E+03
     FCC_A1
  ** GRAPHITE_A9
 Calculated.                      18  equilibria

 Phase region boundary   5 at:   4.561E-01  1.427E+03
  ** LIQUID
     FCC_A1
  ** GRAPHITE_A9

 Phase region boundary   6 at:   8.690E-01  1.427E+03
  ** LIQUID
     FCC_A1
 Calculated.                      15  equilibria

 Phase region boundary   7 at:   9.840E-01  1.768E+03
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary   8 at:   9.939E-01  1.768E+03
  ** BCC_A2
     FCC_A1
 Calculated                      25  equilibria

 Phase region boundary   9 at:   9.858E-01  1.768E+03
     LIQUID
  ** BCC_A2
 Calculated                      20  equilibria

 Phase region boundary  10 at:   4.129E-01  1.427E+03
  ** LIQUID
     GRAPHITE_A9
 Calculated..                      44  equilibria
 Terminating at axis limit.
```

```
 Phase region boundary  11 at:   9.841E-01  1.011E+03
     BCC_A2
  ** FCC_A1
 Calculated                       25  equilibria

 Phase region boundary  12 at:   9.944E-01  1.100E+03
     BCC_A2
  ** FCC_A1
 Calculated                       16  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex01\BINA
 RY.POLY3
 CPU time for mapping                      1  seconds

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes


  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

   ... the command in full is SET_TIELINE_STATUS
   ... the command in full is SET_LABEL_CURVE_OPTION
   ... the command in full is PLOT_DIAGRAM
```

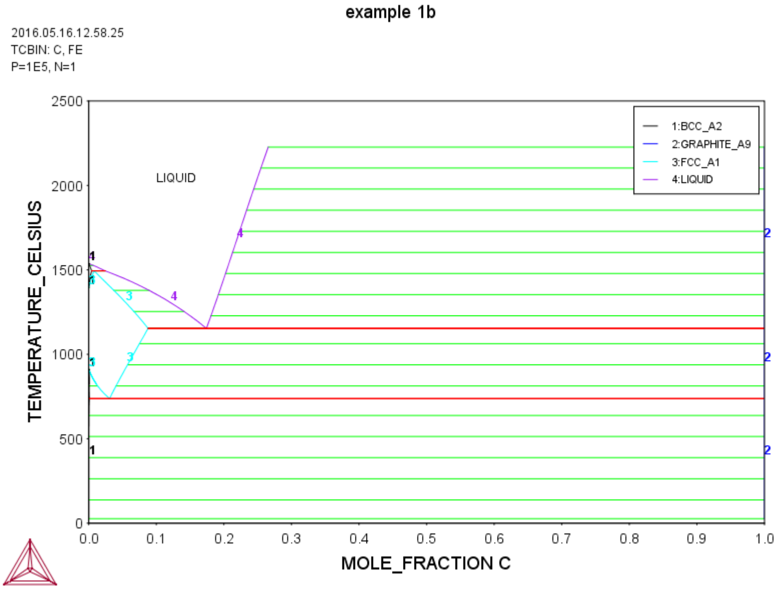


```
POST:
POST:Hit RETURN to continue
POST:
POST: set-title example 1a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

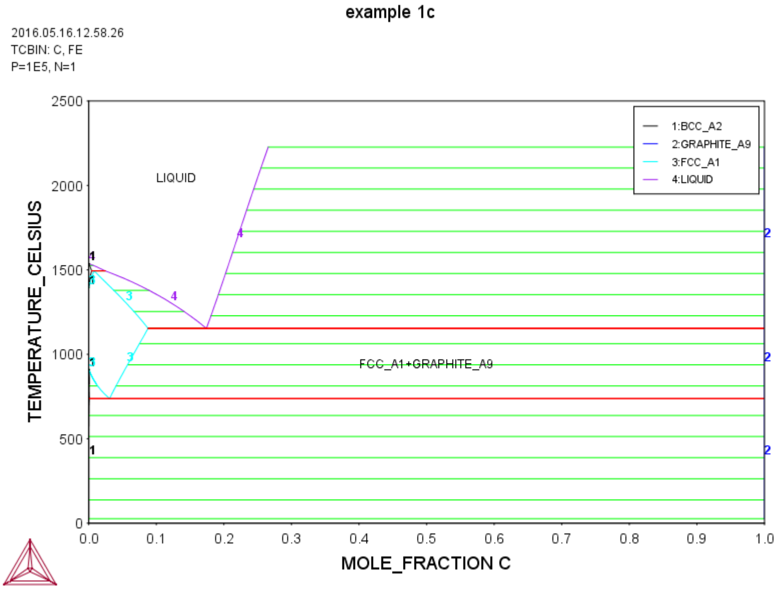


```
POST:
POST:Hit RETURN to continue
POST: @@ By default no label is given, the user must specify it himself.
POST: @@ There are two possibilities, to label the lines or to label the
POST: @@ areas. In the latter case the user must supply a coordinate for the
POST: @@ label, for example
POST: ADD
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .1
Give Y coordinate in axis units: 2000
Automatic phase labels? /Y/: Y
 Automatic labelling not always possible
 Using global minimization procedure
```

```
Calculated           414 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: LIQUID
Text size: /.36/:
POST: set-title example 1b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

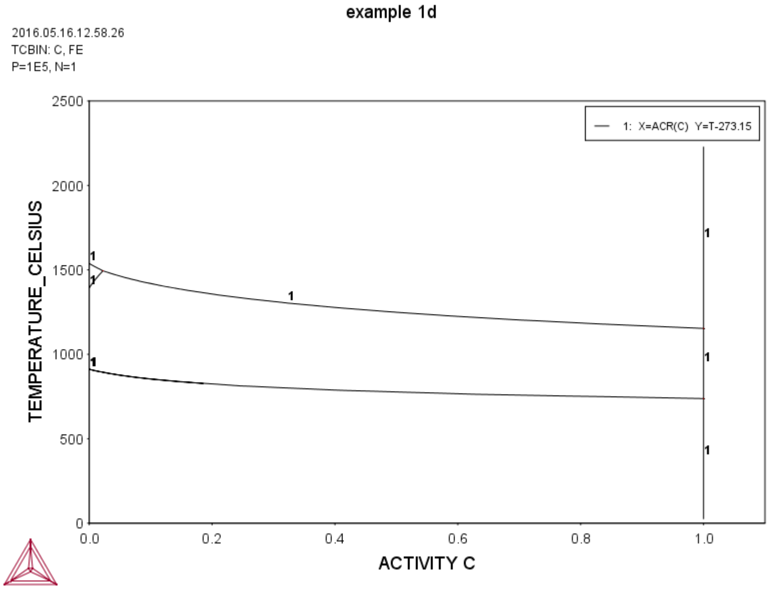


```
POST:
POST:
POST:Hit RETURN to continue
POST: add .4 900
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/: Y
 Automatic labelling not always possible
 Using global minimization procedure
Calculated           414 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: FCC_A1+GRAPHITE_A9
Text size: /.36/:
POST: set-title example 1c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

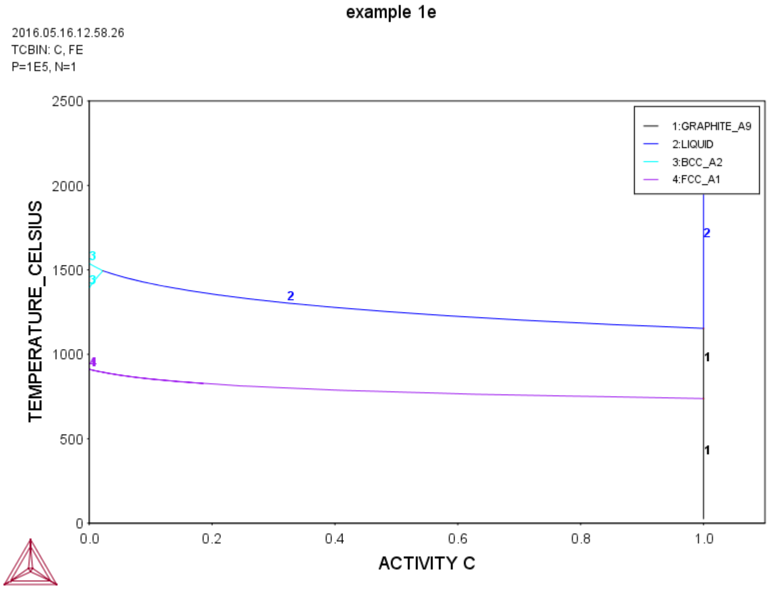


```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ This is the stable phase diagram with graphite and no cementite.
POST: @@ In TC all relevant data from the calculation of the diagram is saved
POST: @@ and it is possible to plot the same diagram using other thermodynamic
POST: @@ quantities, for example replace the carbon composition with its activity
POST: @@ Find out the commands in the post processor by inputing ?
POST: ?
   ... the command in full is HELP
 ADD_LABEL_TEXT            PLOT_DIAGRAM              SET_INTERACTIVE_MODE
 APPEND_EXPERIMENTAL_DATA PRINT_DIAGRAM             SET_LABEL_CURVE_OPTION
 BACK                      QUICK_EXPERIMENTAL_PLOT   SET_PLOT_FORMAT
 CHANGE_LEGEND             REINITIATE_PLOT_SETTINGS SET_PLOT_OPTIONS
 CREATE_3D_PLOTFILE        RESTORE_PHASE_IN_PLOT     SET_PLOT_SIZE
 DUMP_DIAGRAM              SELECT_PLOT               SET_PREFIX_SCALING
 ENTER_SYMBOL              SET_AXIS_LENGTH           SET_RASTER_STATUS
 EXIT                      SET_AXIS_PLOT_STATUS      SET_REFERENCE_STATE
 FIND_LINE                 SET_AXIS_TEXT_STATUS      SET_SCALING_STATUS
 HELP                      SET_AXIS_TYPE             SET_TIC_TYPE
 LIST_DATA_TABLE           SET_COLOR                 SET_TIELINE_STATUS
 LIST_PLOT_SETTINGS        SET_CORNER_TEXT           SET_TITLE
```

```
 LIST_SYMBOLS              SET_DIAGRAM_AXIS          SET_TRUE_MANUAL_SCALING
 MAKE_EXPERIMENTAL_DATAFI SET_DIAGRAM_TYPE          SUSPEND_PHASE_IN_PLOT
 MODIFY_LABEL_TEXT         SET_FONT                  TABULATE
POST: @@ The command to set axis for the diagram is SET-DIAGRAM-AXIS
POST: s-d-a x
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
 UNKNOWN QUESTION VARIABLE :
VARIABLE : ac
FOR COMPONENT : c
POST: set-title example 1d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ The diagram stops at unit activity which represent graphite.
POST: @@ The labels disappear when one sets a new diagram axis because they
POST: @@ are relative to the axis values, not the axis quantities.
POST: @@
POST: @@ A simpler way to identify the stable phases is to use
POST: @@ the command set-label
POST: set-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: ?
 THE OPTIONS MEANS:
 A      LIST STABLE PHASES ALONG LINE
 B      AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
 C      LIST AXIS QUANTITIES
 D      AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
 E      AS B WITH CHANGING COLORS
 F      AS D WITH CHANGING COLORS
 N      NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: B
POST: set-title example 1e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ The metastable diagram, with cementite, can also be calculated but then
POST: @@ one must do some manipulations in POLY. We can use the data
POST: @@ we already retrieved from the database.
POST: back
 Current database: Steels/Fe-Alloys  v8.0
```

```
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
SYS: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ The BIN module has used the poly-3 workspace to calculate the
POLY_3: @@ diagram. We have all data available here. The workspace has been
POLY_3: @@ saved on a file and we can read this back with the command READ.
POLY_3:
POLY_3: read,,,
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: @@ There are many command in the POLY module. They make it possible
POLY_3: @@ to calculate almost any kind of equilibrium and diagram.
POLY_3: @@ With the ? we can list all commands
POLY_3: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  EXIT                     REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE              SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                     SELECT_EQUILIBRIUM
 BACK                     INFORMATION              SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE       SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS          SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM         SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA  SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS              SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS             SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN          SET_START_VALUE
 DELETE_SYMBOL            MAP                      SHOW_VALUE
 ENTER_SYMBOL             POST                     STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES          TABULATE
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ More information about a command can be obtaind with the HELP command
POLY_3: help
COMMAND: list-status

 LIST_STATUS

 The status of components, species or phases can be listed with this command.
 The user may select all or some of these.

 Synopsis 1:     LIST_STATUS <keyword(s)>
 Synopsis 2:     LIST_STATUS
 Ensuing Prompt: Option /CPS/: <keyword(s)>

 Keyword = C   means list component status
           P   means list phase status
           S   means list species status

 Default is CPS. By pressing <RETURN>, a complete list with status for
 components, phases and species is obtained. By just giving P, a list
 of just the phase statuses is obtained. If you are also interested in
 component status, then type C. You may also simply input CS so that
 a list of statuses for both components and species can be listed out.

 The statuses of components, phases and species can be changed with the
 CHANGE_STATUS command.

 Results: Depending upon the key word specified in the CHANGE_STATUS options,
  a table with the current statuses of phases or species or components, or
  their combinations, is shown up.
  * For components, their statuses and reference states are listed.
  * For ENTERED and FIXED phases, their statuses, driving forces and
      equilibrated amount (of stable) are listed. Note that the metastable
      phases are listed in descending order of stability. To avoid long
      outputs, in the versions later than version N, only 10 metastable
      phases (in ENTERED status) will be listed by lines, while all other
      less stable phases are merged onto one line. For DORMANT phases,
      their phase names and driving forces are listed. For SUSPENDED phases,
      only the phase names are listed into one line.
  * For species, only the status are listed out.

  Example:
   POLY_3:l-st
   Option /CPS/:
   *** STATUS FOR ALL COMPONENTS
   COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
   VA                      ENTERED   SER
   C                       ENTERED   GRAPHITE       *              *
   FE                      ENTERED   SER
   NI                      ENTERED   SER
   *** STATUS FOR ALL PHASES
   PHASE                   STATUS    DRIVING FORCE   MOLES
   FCC_A1                  FIXED      0.00000000E+00  1.00000000E+00
   BCC_A2                  ENTERED    0.00000000E+00  0.00000000E+00
   HCP_A3                  ENTERED   -2.69336869E-01  0.00000000E+00
   CEMENTITE               ENTERED   -2.86321394E-01  0.00000000E+00
   M23C6                   ENTERED   -3.44809821E-01  0.00000000E+00
   LIQUID                  ENTERED   -4.95421844E-01  0.00000000E+00
   CBCC_A12                ENTERED   -6.16764645E-01  0.00000000E+00
   M7C3                    ENTERED   -6.56332559E-01  0.00000000E+00
   M5C2                    ENTERED   -6.83594326E-01  0.00000000E+00
   GRAPHITE                ENTERED   -1.02142788E+00  0.00000000E+00
   DIAMOND_A4              ENTERED   -1.73225646E+00  0.00000000E+00
   ALNI_B2                 ENTERED   -4.79816887E+00  0.00000000E+00
   ENTERED PHASES WITH DRIVING FORCE LESS THAN    -4.80
   AL3NI2 GAS
   HCP_A3                  DORMANT   -2.69336869E-01
   SUSPENDED PHASES:
   V3C2 KSI_CARBIDE FECN_CHI FE4N CUB_A13
   *** STATUS FOR ALL SPECIES
   C  ENTERED    C2 ENTERED    C4 ENTERED    C6 ENTERED    FE ENTERED
   C1 ENTERED    C3 ENTERED    C5 ENTERED    C7 ENTERED    NI ENTERED
   VA ENTERED

 The statuses of components, phases and species can be changed with the
 CHANGE_STATUS command.


POLY_3:Hit RETURN to continue
POLY_3: @@ General information can be obtained using the INFORMATION command
POLY_3: INFO
```

```
   ... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/:
 PURPOSE

         INTRODUCTION to the Equilibrium Calculation Module (POLY)
        ***********************************************************

 Knowledge of the thermodynamic equilibrium is an important factor for
 understanding properties of materials and processes. With a database of
 thermodynamic model parameters, it is possible to predict such properties
 and also to obtain driving forces for diffusion-controlled phase
 transformations and other dynamic processes.

 With the comprehensive Equilibrium Calculation module, POLY ? it is possible
 to calculate many different kinds of equilibria and diagrams, in particular
 multicomponent phase diagrams. This is thus an important tool in developing
 new materials and processes. The current POLY module is its third version;
 this is why is often referred as POLY_3 in the Thermo-Calc software.

 Different kind of databases can be used with the POLY module, and thus it
 can be used for alloys or ceramic system, as well as gaseous equilibria,
 aqueous solution involved heterogeneous interaction systems. Since TCCN,
 up to 40 elements and 1000 species can be defined into a single system
 (previously 20 elements and 400 species) for equilibrium calculations.

 Great care has been taken to provide the users with the most flexible tool.
 All normal thermodynamic state variables can be used to set as conditions in
 calculating equilibria, and as axes in plotting diagrams. A unique facility
 is to set the composition or any property of an individual phase as a
 condition. Any state variable can be varied along an axis in order to
 generate a diagram. During calculations of a diagram, complete descriptions
 of all calculated equilibria are stored, and in the diagram any state
 variable can be used as axis.

 One of the major improvements since the TCCR/TCW4 software version is that
 the recently-implemented Global Minimization Technique is used to assure
 that the present minimum in an equilibrium calculation is the most stable
 minima for the specified conditions. This new technique, which is based
 on the traditional GEM (Gibbs Energy Minimization) Technique (i.e., the
 ordinary POLY Minimization routines used in previous versions, where
 pre-knowledge of miscibility gaps in involved phases are necessary,
 otherwise, metastable equilibria instead of the stable equilibria may be
 obtained), will ultimately prevent a calculation from reaching an undesired
 metastable or unstable (local) equilibrium in a defined system, and
 automatically detect possible miscibility gap(s) and automatically create
 additional composition sets in a solution phase if needed for handling
 single or multiple miscibility gaps. Therefore it is no longer necessary
 for the user to specify additional composition sets in advance.

 A Direct Global Minimization can be performed on conditions: N, n(comp),
 B, b(comp), w(comp), x(comp), T, and P, but not when combined conditions
 as e.g. w(a)-3*w(b)=1 are used or when an activity or potential condition
 is used. For all other types of conditions where regular minimization
 converges, Indirect Global Minimization, i.e. global test and corrections,
 if necessary, are performed until the lowest minimum is found.

  * Direct Global Minimization: From the mesh of Gibbs energy, find the set
    of grid points that gives the lowest energy solution under the specified
    conditions. This set of grid points provides starting combination of
    phases and their constitutions for regular minimization to find the
    exact equilibrium solution. This solution will be then subject to a
    global test as described below.

  * Indirect Global Minimization: Under certain conditions, direct approach
    is impossible. In this case, regular minimization is performed first
    and then a check is performed in order to see if the found local minimum
    is a global one by checking if all grid points are above the equilibrium
    Gibbs energy plane. If not, then recalculate by including these grid
    points until no grid point is above the equilibrium Gibbs energy plane
    from the previous step.

 The full-scale and full-scope usage of the Global Minimization Technique has
 been extended from for only single-point calculations within TCCR/TCW4 to
 for all types of calculations (of single-points, property diagram stepping
 and phase diagram mapping) within TCCS/TCW5.

 The use of Global Minimization Technique may increase the computation time,
 while it is not an issue at all, thanks for the rapid developments of
 computer hardware nowadays.

  * The main cost in time comes from the calculation of Gibbs energy at each
    grid point generated by properly meshing the composition space for each
    entered phase. In a typical multicomponent system calculation, about
    100MB of RAM memory is needed in storing the mesh of Gibbs energies.

  * An additional (but much smaller) cost in time comes from finding the set
    of grid points in the above mesh that give the lowest energy solution.
    This solution is where POLY starts its ordinary minimization. When POLY
    has found an equilibrium, the equilibrium Gibbs energy surface is
    compared to the mesh to assure that no grid point is below the surface,
    i.e. a global minimization has been reached.

 Global Minimization is now performed by default in single-point or
 stepping or mapping equilibrium calculations, but can of course be
 turned off (and on again by repeating the command-sequence of
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION) by the user for specific purposes.
 This means that truly stable equilibrium should be guaranteed for
 single-points, stepping and mapping calculations.
  * A completely new stepping and mapping procedure that ensures Global
    Minimization everywhere it is critical has been developed and been
    made available in TCCS/TCW5. These newly re-written STEP/MAP routines
    are very important for stepping/mapping calculations in multicomponent
    systems where there are complex miscibility gaps in some phases, and
    it does not require having any ??good?? guess of starting points.
    Therefore, TCCS/TCW5 can automatically handle complex solution phases
    with single or multiple miscibility gaps  [for instance, a solution
    phase that is thermodynamically described as a single phase in a
    Thermo-Calc database, such as FCC, BCC or HCP phases, may be split
    into two or several composition-sets/phases that are presented in
    an equilibrium state as metallic phase(s), carbide(s), nitride(s),
    carbonitride(s), nitrocarbide(s), and so on], and can thus ensure
    the correct and complete phase diagrams and property diagrams in
    multicomponent systems, without bothering staring points.

 Together with the PARROT module, the POLY module is also used for critical
 assessment of experimental data in order to develop thermodynamic databases.
```

```
 The POLY module uses the Gibbs Energy System (GES) for modeling and data
 manipulations of the thermodynamic properties of each phase.

 The following commands are available in the POLY module:
 POLY_3:?
  ADD_INITIAL_EQUILIBRIUM  EXIT                     REINITIATE_MODULE
  ADVANCED_OPTIONS         GOTO_MODULE              SAVE_WORKSPACES
  AMEND_STORED_EQUILIBRIA  HELP                     SELECT_EQUILIBRIUM
  BACK                     INFORMATION              SET_ALL_START_VALUES
  CHANGE_STATUS            LIST_AXIS_VARIABLE       SET_AXIS_VARIABLE
  COMPUTE_EQUILIBRIUM      LIST_CONDITIONS          SET_CONDITION
  COMPUTE_TRANSITION       LIST_EQUILIBRIUM         SET_INPUT_AMOUNTS
  CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA  SET_INTERACTIVE
  DEFINE_COMPONENTS        LIST_STATUS              SET_NUMERICAL_LIMITS
  DEFINE_DIAGRAM           LIST_SYMBOLS             SET_REFERENCE_STATE
  DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
  DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN          SET_START_VALUE
  DELETE_SYMBOL            MAP                      SHOW_VALUE
  ENTER_SYMBOL             POST                     STEP_WITH_OPTIONS
  EVALUATE_FUNCTIONS       READ_WORKSPACES          TABULATE
 POLY_3:

 Note that, since TCCS, the SPECIAL_OPTIONS and SET_MINIMIZAION_OPTIONS
 commands (the later one was introduced in the TCCR version) has been merged
 into the new ADVANCED_OPTIONS command; and the RECOVER_START_VALUES command
 has been removed, due to that is not relevant to the POLY module anymore.

 Revision History of the POLY-Module User's Guide:
 ==================================================
  Mar 1991  First release
                  (Edited by Bo Jansson and Bo Sundman)
  Oct 1993  Second revised release (with version J)
                  (Edited by Bo Jansson and Bo Sundman)
  Oct 1996  Third revised release (with version L)
                  (Edited by Bo Sundman)
  Nov 1998  Fourth revised release (with version M)
                  (Edited by Bo Sundman)
  Jun 2000  Fifth revised and extended release
                  (Edited by Pingfang Shi)
  Nov 2002  Sixth revised and extended release
                  (Edited by Pingfang Shi)
  May 2006  Eighth revised and extended release
                  (Edited by Pingfang Shi)
  Apr 2008  Ninth revised and extended release
                  (Edited by Pingfang Shi)
```

WHICH SUBJECT: ?

```
 WHICH SUBJECT

 Specify a subject (or its abbreviation as long as it is unique, e.g.,
 SIN, SIT, SOL, SPE, STATE, STEP, SYM, SYS, SUB, etc.) on which information
 should be given, from the following subjects that are important to the use
 of the POLY module:

  PURPOSE                GETTING STARTED          USER INTERFACE
  HELP                   MACRO FACILITY           PRIVATE FILES
  BASIC THERMODYNAMICS   SYSTEM AND PHASES        CONSTITUENTS AND SPECIES
  SUBLATTICES            COMPONENTS               SITE AND MOLE FRACTIONS
  COMPOSITION AND CONSTITUTION                    CONCENTRATION
  STATE VARIABLES        INTENSIVE VARIABLES      EXTENSIVE VARIABLES
  DERIVED VARIABLES      UNITS                    BASIC UNITS
  SYSTEM UNITS           COMPONENT UNITS          PHASE UNITS
  PHASE-COMPONENT UNITS  PHASE-SPECIES UNITS      USER-SPECIFIED UNITS
  SYMBOLS                REFERENCE STATES         METASTABLE EQUILIBRIUM
  CONDITIONS             AXIS-VARIABLES           SPECIAL OPTIONS
  CALCULATIONS TYPES     SINGLE EQUILIBRIUM       INITIAL EQUILIBRIUM
  STEPPING               SOLIDIFICATION PATH      PARAEQUILIBRIUM AND T0
  MAPPING                PLOTTING OF DIAGRAMS     GLOBAL MINIMIZATION
  DIAGRAM TYPES          BINARY DIAGRAMS          TERNARY DIAGRAMS
  QUASI-BINARY DIAGRAMS  HIGHER ORDER DIAGRAMS    PROPERTY DIAGRAMS
  POTENTIAL DIAGRAMS     POURBAIX DIAGRAMS        AQUEOUS SOLUTIONS
  ORDER-DISORDER         TROUBLE SHOOTING         FAQ

 If you are using the ED_EXP module (the sub-module of the PARROT module),
 you can also get detailed information of the following subject keywords
 which are relevant to the EX_EXP module:

  EDEXP     for Edit-Experiment Module (ED-EXP)
  EDPOLY    for Performance of POLY Commands in the ED_EXP Module
  EDSPECIAL for Special Commands only available in the ED_EXP Module
  EDPOP     for Other Commands in the Experimental Data (POP or DOP) Files
```

WHICH SUBJECT: state

```
 STATE VARIABLES

             Standard State Variables and Partial Derivatives
        ************************************************************

 Classic Thermodynamics deals only with systems that are in equilibrium,
 i.e., in an EQUILIBRIUM STATE (either as full equilibrium, or partial or
 local equilibrium) which is stable against internal fluctuations in a
 number of variables, such as temperature and composition. These variables
 that have defined values or properties at the equilibrium state are called
 STATE VARIABLES. Other examples of state variables are pressure (P),
 and chemical potential (m). Thermodynamics provides a number of relations
 between these state variables that make it possible to calculate the value
 of any other variable at equilibrium.

 A state variable can be of two types, extensive or intensive. The value
 of an extensive variable, e.g., volume, depends on the size of the system,
 whereas the value of an intensive variable, e.g., temperature, is independent
 of the size of the system. Each type of state variable has a complementary
 variable of the other type. The variable complementing the volume is
 pressure, while the variable complementing the composition of a component
 is its chemical potential.

 It is worth mentioning here that the activity of a component can always
 be obtained from its chemical potential using a simple mathematical
 relationship. It is also possible to choose any convenient reference state
 for the activity or the chemical potential. One of the advantages with a
 thermodynamic databank on a computer is that, in most cases, such reference
 state changes can be handled internally without troubling the user.
```

```
 If the work that can be exchanged with the surroundings is limited to
 pressure-volume work, the state of equilibrium of a system can be obtained
 by assigning values to exactly N+2 state variables where N is the number
 of components of the system.

 Note that the Thermo-Calc software distinguishes between components of a
 system and constituent (i.e., species) of a phase in the system. Many state
 variables require one or the other. By default, the elements are defined
 as the system components, but this definition can be changed with the POLY
 command DEFINE_COMPONENT. For instance, if the elements are Ca, Si and O,
 the another set of components can be defined as CaO, SiO and O2; in a pure
 water system, the components are normally defined as H2O and H+. However,
 one can not change the number of components when using this command.

 A state variable is a defined thermodynamic quantity either for the whole
 system, or for a component in the system, or a species in a specific
 substitutional phase, or a constituent (i.e., a species on a specific
 sublattice site) in a specific solution phase.

 The POLY module operates on a thermodynamic system in a stable or meta-stable
 or partial/local equilibrium state that is described by state variables.
 Examples of state variables are temperature, mole fraction, chemical
 potential and activity of a component (in the system or in a specific
 phase), enthalpy (of the system or a specific phase), etc. In the POLY
 module, a general notational method has been designed for the important
 set of standard state variables and their partial derivatives (or called
 as derived variables).

 Common examples of state variables in a defined system are:
  T               for temperature (K)
  P               for pressure (Pa)
  N               for total system size (in moles)
  B               for total system site (in grams)
  N(H)            for overall mole number of the hydrogen component
  B(H2O)          for overall mass (grams) of the H2O component
  X(FE)           for overall mole fraction of the FE component
  W(AL2O3)        for overall mass fraction of the AL2O3 component
  Y(HCP,CR#1)     for site fraction of the Cr species
                            on the first sublattice site in the HCP phase
  X(LIQUID,FE)    for mole fraction of the Fe component in the LIQUID phase
  W(FCC,C)        for mass fraction of the C component in the FCC phase
  NP(BCC)         for mole number of the BCC phase
  BP(BCC)         for mass (grams) of the BCC phase
  VP(BCC)         for volume (m3) of the BCC phase
  DGM(BCC)        for driving force of the BCC phase per mole of components
  QF(SIGMA)       for phase stability function of the SIGMA phase
  MUR(C)          for chemical potential of the C component
                            (with regard to its reference state)
  ACR(C)          for activity of the C component
                            (with regard to its reference state)
  LNACR(C)        fatural logarithm of activity of the C component
                            [lnACR(C)=MUR(C)/RT]
  MUR(FE+3,AQ)    for chemical potential of the Fe+3 species
                            related to the aqueous solution phase
  ACR(FE+3,AQ)    for activity of the Fe+3 species
                            related to the aqueous solution phase
  LNACR(FE+3,AQ)  for natural logarithm of activity of the Fe+3 species
                            related to the aqueous solution phase
                            [lnACR(FE+3,AQ)=MUR(FE+3,AQ)/RT]
  HM              for total enthalpy per mole component in the system
  HM(FCC)         for enthalpy per mole component of the FCC phase
  HM.T            for heat capacity per mole of components
                            in the system (in J/mol/K)
  HM(FCC).T       for heat capacity per mole of components
                            of the FCC phase (in J/mol/K)
  P.T             for the slope delta_P/delta_T of a phase boundary
                            on a P-T phase diagram. Note that the equilibrium
                            with a phase assemblage must have been calculated.
  T.W(SI)         for the slope delta_T/delta_W(Si) of a phase boundary
                            on a T-W(Si) phase diagram with regard to
                            mass of the component in the system
  T.X(LIQ,CR)     for the slope delta_T/delta_X(Liq,Cr) of a phase boundary
                            on a T-X(Liq,Cr) phase diagram with regard to
                            mole fraction of the component in the phase

   Many more ?     >>> see details below and in the document of
                                  Thermo-Calc Software System
                                  ***************************

 Note that the state variables involving components can be used for the
 defined components, but not for any species. To define new components
 in a defined system, the DEFINE_COMPONENT command should be used.

 The basic intensive and extensive variables which are suitable in the
 POLY module of in the Thermo-Calc software system are listed and briefly
 described in Table 1 (of the document Thermo-Calc Software System), and
 are also be dealt with in the following subject-keywords when using the
 on-line help feature of the POLY module:
   INFO INTENSIVE VARIABLES    For Various Intensive State Variables
   INFO EXTENSIVE VARIABLES    For Various Extensive State Variables

 Derivatives of state variables can be evaluated using a dot "." between
 two state variables. Many derived variables of a defined system, or of
 a certain system component, or of a given phase, or of a specific component
 in a defined phase, can be easily obtained using appropriate partial
 derivatives of state variables, such as heat capacity, thermal expansivity,
 isothermal compressibility, among others. For the details of various
 derived variables which are suitable in the POLY and POST modules of the
 Thermo-Calc software system, please refer to Section 2.6 in the document
 Thermo-Calc Software System, and also refer to the on-line help feature
 of the POLY module:
   INFO DERIVED VARIABLES      For Derived Variables (Partial Derivatives)

 Note that the lists of various state variables in the subject-keywords
 INTENSIVE VARIABLES and EXTENSIVE VARIABLES, as well as of derived variables
 (partial derivatives), are not exhaustive, but many other remaining state
 variables can be obtained through direct calls or by using combinations of
 the predefined state variables (such as those listed in the subject-keyword
 DERIVED VARIABLES (for various derived variables or partial derivatives)
 or user-specified ones. For more details, please refer to Sections 2.5
 [Equilibrium State and State Variables] and 2.6 [Derived Variables (Partial
 Derivatives)] in the document Thermo-Calc Software System.


WHICH SUBJECT:
POLY_3:Hit RETURN to continue
```

```
POLY_3: @@ We can list the current equilibrium by
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: ?

 OPTIONS

   The user may select the output units and formats by optionally specifying
   a combination of the following letters:
     Fraction order:   V means VALUE ORDER
                       A means ALPHABETICAL ORDER
     Fraction type:    W means MASS FRACTION
                       X means MOLE FRACTION
     Composition:      C means only COMPOSITION
                       N means CONSTITUTION and COMPOSITION.
     Phase:            S means including only STABLE PHASES
                       P means including ALL NON-SUSPENDED PHASES.

   Default is VWCS. If the output should be in mole fraction, then give
   VXCS or just X.


Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCBIN

 Conditions:
 X(FE)=0.99, P=1E5, N=1, T=1100
 DEGREES OF FREEDOM 0

 Temperature   1100.00 K (   826.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.54086E+01
 Total Gibbs energy -4.90502E+04,  Enthalpy  3.18534E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.0000E-02  2.1677E-03 1.8555E-01 -1.5406E+04 GRAPHITE
 FE                      9.9000E-01  9.9783E-01 9.9957E-01 -3.9762E+00 BCC_A2

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.97662E-01  C   2.33819E-03

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.99907E-01  C   9.33835E-05
POLY_3:Hit RETURN to continue
POLY_3: @@ The actual conditions are listed by the list-equil command but
POLY_3: @@ can be obtained also by
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 X(FE)=0.99, P=1E5, N=1, T=1100
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ The meaning of the state variables T, P, X, N  and many others
POLY_3: @@ are explained by the INFO command
POLY_3: INFO
   ... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/: state
 STATE VARIABLES

              Standard State Variables and Partial Derivatives
         ***********************************************************

 Classic Thermodynamics deals only with systems that are in equilibrium,
 i.e., in an EQUILIBRIUM STATE (either as full equilibrium, or partial or
 local equilibrium) which is stable against internal fluctuations in a
 number of variables, such as temperature and composition. These variables
 that have defined values or properties at the equilibrium state are called
 STATE VARIABLES. Other examples of state variables are pressure (P),
 and chemical potential (m). Thermodynamics provides a number of relations
 between these state variables that make it possible to calculate the value
 of any other variable at equilibrium.

 A state variable can be of two types, extensive or intensive. The value
 of an extensive variable, e.g., volume, depends on the size of the system,
 whereas the value of an intensive variable, e.g., temperature, is independent
 of the size of the system. Each type of state variable has a complementary
 variable of the other type. The variable complementing the volume is
 pressure, while the variable complementing the composition of a component
 is its chemical potential.

 It is worth mentioning here that the activity of a component can always
 be obtained from its chemical potential using a simple mathematical
 relationship. It is also possible to choose any convenient reference state
 for the activity or the chemical potential. One of the advantages with a
 thermodynamic databank on a computer is that, in most cases, such reference
 state changes can be handled internally without troubling the user.

 If the work that can be exchanged with the surroundings is limited to
 pressure-volume work, the state of equilibrium of a system can be obtained
 by assigning values to exactly N+2 state variables where N is the number
 of components of the system.

 Note that the Thermo-Calc software distinguishes between components of a
 system and constituent (i.e., species) of a phase in the system. Many state
 variables require one or the other. By default, the elements are defined
 as the system components, but this definition can be changed with the POLY
 command DEFINE_COMPONENT. For instance, if the elements are Ca, Si and O,
 the another set of components can be defined as CaO, SiO and O2; in a pure
 water system, the components are normally defined as H2O and H+. However,
 one can not change the number of components when using this command.

 A state variable is a defined thermodynamic quantity either for the whole
 system, or for a component in the system, or a species in a specific
 substitutional phase, or a constituent (i.e., a species on a specific
 sublattice site) in a specific solution phase.

 The POLY module operates on a thermodynamic system in a stable or meta-stable
 or partial/local equilibrium state that is described by state variables.
 Examples of state variables are temperature, mole fraction, chemical
 potential and activity of a component (in the system or in a specific
 phase), enthalpy (of the system or a specific phase), etc. In the POLY
 module, a general notational method has been designed for the important
 set of standard state variables and their partial derivatives (or called
```

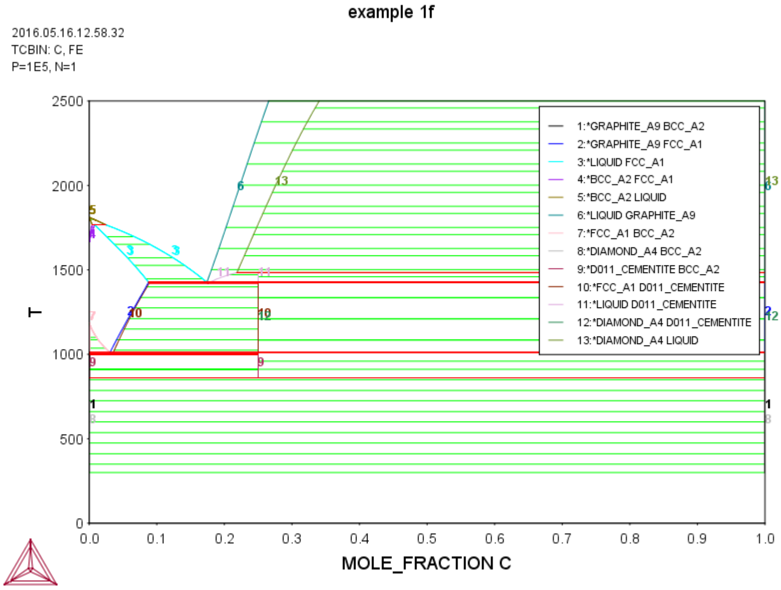
```
 as derived variables).

 Common examples of state variables in a defined system are:
  T               for temperature (K)
  P               for pressure (Pa)
  N               for total system size (in moles)
  B               for total system site (in grams)
  N(H)            for overall mole number of the hydrogen component
  B(H2O)          for overall mass (grams) of the H2O component
  X(FE)           for overall mole fraction of the FE component
  W(AL2O3)        for overall mass fraction of the AL2O3 component
  Y(HCP,CR#1)     for site fraction of the Cr species
                            on the first sublattice site in the HCP phase
  X(LIQUID,FE)    for mole fraction of the Fe component in the LIQUID phase
  W(FCC,C)        for mass fraction of the C component in the FCC phase
  NP(BCC)         for mole number of the BCC phase
  BP(BCC)         for mass (grams) of the BCC phase
  VP(BCC)         for volume (m3) of the BCC phase
  DGM(BCC)        for driving force of the BCC phase per mole of components
  QF(SIGMA)       for phase stability function of the SIGMA phase
  MUR(C)          for chemical potential of the C component
                            (with regard to its reference state)
  ACR(C)          for activity of the C component
                            (with regard to its reference state)
  LNACR(C)        fatural logarithm of activity of the C component
                            [lnACR(C)=MUR(C)/RT]
  MUR(FE+3,AQ)    for chemical potential of the Fe+3 species
                            related to the aqueous solution phase
  ACR(FE+3,AQ)    for activity of the Fe+3 species
                            related to the aqueous solution phase
  LNACR(FE+3,AQ)  for natural logarithm of activity of the Fe+3 species
                            related to the aqueous solution phase
                            [lnACR(FE+3,AQ)=MUR(FE+3,AQ)/RT]
  HM              for total enthalpy per mole component in the system
  HM(FCC)         for enthalpy per mole component of the FCC phase
  HM.T            for heat capacity per mole of components
                            in the system (in J/mol/K)
  HM(FCC).T       for heat capacity per mole of components
                            of the FCC phase (in J/mol/K)
  P.T             for the slope delta_P/delta_T of a phase boundary
                            on a P-T phase diagram. Note that the equilibrium
                            with a phase assemblage must have been calculated.
  T.W(SI)         for the slope delta_T/delta_W(Si) of a phase boundary
                            on a T-W(Si) phase diagram with regard to
                            mass of the component in the system
  T.X(LIQ,CR)     for the slope delta_T/delta_X(Liq,Cr) of a phase boundary
                            on a T-X(Liq,Cr) phase diagram with regard to
                            mole fraction of the component in the phase

   Many more ?     >>> see details below and in the document of
                                   Thermo-Calc Software System
                                   ***************************

 Note that the state variables involving components can be used for the
 defined components, but not for any species. To define new components
 in a defined system, the DEFINE_COMPONENT command should be used.

 The basic intensive and extensive variables which are suitable in the
 POLY module of in the Thermo-Calc software system are listed and briefly
 described in Table 1 (of the document Thermo-Calc Software System), and
 are also be dealt with in the following subject-keywords when using the
 on-line help feature of the POLY module:
   INFO INTENSIVE VARIABLES    For Various Intensive State Variables
   INFO EXTENSIVE VARIABLES    For Various Extensive State Variables

 Derivatives of state variables can be evaluated using a dot "." between
 two state variables. Many derived variables of a defined system, or of
 a certain system component, or of a given phase, or of a specific component
 in a defined phase, can be easily obtained using appropriate partial
 derivatives of state variables, such as heat capacity, thermal expansivity,
 isothermal compressibility, among others. For the details of various
 derived variables which are suitable in the POLY and POST modules of the
 Thermo-Calc software system, please refer to Section 2.6 in the document
 Thermo-Calc Software System, and also refer to the on-line help feature
 of the POLY module:
   INFO DERIVED VARIABLES      For Derived Variables (Partial Derivatives)

 Note that the lists of various state variables in the subject-keywords
 INTENSIVE VARIABLES and EXTENSIVE VARIABLES, as well as of derived variables
 (partial derivatives), are not exhaustive, but many other remaining state
 variables can be obtained through direct calls or by using combinations of
 the predefined state variables (such as those listed in the subject-keyword
 DERIVED VARIABLES (for various derived variables or partial derivatives)
 or user-specified ones. For more details, please refer to Sections 2.5
 [Equilibrium State and State Variables] and 2.6 [Derived Variables (Partial
 Derivatives)] in the document Thermo-Calc Software System.


WHICH SUBJECT:
POLY_3:Hit RETURN to continue
POLY_3: @@ The use of state variables as conditions is the key to the
POLY_3: @@ flexibility of TC. Each condition is set independently and
POLY_3: @@ any condition can be set as axis variable.
POLY_3: @@
POLY_3: @@ Now we just want to take away the graphite in order to calculate the
POLY_3: @@ metastable Fe-C diagram with cementite. We can list all phases by the
POLY_3: @@ LIST_STATUS command
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 C                        ENTERED   GRAPHITE_A9    *              100000
 FE                       ENTERED   BCC_A2         *              100000
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    9.246266E-01
 BCC_A2                   ENTERED      0.000000E+00    7.537335E-02
 D011_CEMENTITE           ENTERED     -4.153716E-01    0.000000E+00
 LIQUID                   ENTERED     -4.668963E-01    0.000000E+00
 GRAPHITE_A9              ENTERED     -1.684424E+00    0.000000E+00
 DIAMOND_A4               ENTERED     -2.386932E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 C    ENTERED    C3   ENTERED    FE   ENTERED    VA   ENTERED
```

```
 C1   ENTERED    C4   ENTERED    FE+2 ENTERED    VA-2 ENTERED
 C2   ENTERED    C5   ENTERED    FE+3 ENTERED    VA-4 ENTERED
POLY_3:Hit RETURN to continue
POLY_3: @@ The status is changed by the CHANGE_STATUS command
POLY_3: ch-st
   ... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): ?

 Phase name(s)

  In case of "phase" as the keyword, the names of the phases that shall
  have their status changes must be given (all on one line). A comma or
  space must be used as separator. The status to be assigned to the phases
  can also be given on the same line if preceded with an equal sign "=".
  Note that an asterisk, "*", can be used to denote all phases. The special
  notations "*S", i.e., a * directly followed by an S, means all suspended
  phases. In the same way, "*D" means all dormant phases, and "*E" means
  all entered phases.


Phase name(s): gra
Status: /ENTERED/: sus
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 C                        ENTERED   GRAPHITE_A9    *              100000
 FE                       ENTERED   BCC_A2         *              100000
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    9.246266E-01
 BCC_A2                   ENTERED      0.000000E+00    7.537335E-02
 D011_CEMENTITE           ENTERED     -4.153716E-01    0.000000E+00
 LIQUID                   ENTERED     -4.668963E-01    0.000000E+00
 DIAMOND_A4               ENTERED     -2.386932E+00    0.000000E+00
 SUSPENDED PHASES:
 GRAPHITE_A9
 *** STATUS FOR ALL SPECIES
 C    ENTERED    C3   ENTERED    FE   ENTERED    VA   ENTERED
 C1   ENTERED    C4   ENTERED    FE+2 ENTERED    VA-2 ENTERED
 C2   ENTERED    C5   ENTERED    FE+3 ENTERED    VA-4 ENTERED
POLY_3:Hit RETURN to continue
POLY_3: @@ Note that the graphite is listed as suspended this time.
POLY_3: @@ we try to calculate the equilibrium without graphite.
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           413 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ A number of ,,, after a command means to accept default values.
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCBIN

 Conditions:
 X(FE)=0.99, P=1E5, N=1, T=1100
 DEGREES OF FREEDOM 0

 Temperature   1100.00 K (   826.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.54086E+01
 Total Gibbs energy -4.90502E+04,  Enthalpy  3.18534E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        1.0000E-02  2.1677E-03 1.8555E-01 -1.5406E+04 GRAPHITE
 FE                       9.9000E-01  9.9783E-01 9.9957E-01 -3.9762E+00 BCC_A2

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.97662E-01  C   2.33819E-03

 BCC_A2                       Status ENTERED     Driving force  0.0000E+00
 Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.99907E-01  C   9.33835E-05
POLY_3:Hit RETURN to continue
POLY_3: @@ It may seem surprising that diamond is stable but the total mole fraction
POLY_3: @@ of iron is less than 0.5, so we are on the carbon rich side
POLY_3: @@ of cementite, and it is reasonable.
POLY_3:
POLY_3: @@ Now try to map the metastable diagram now
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
```

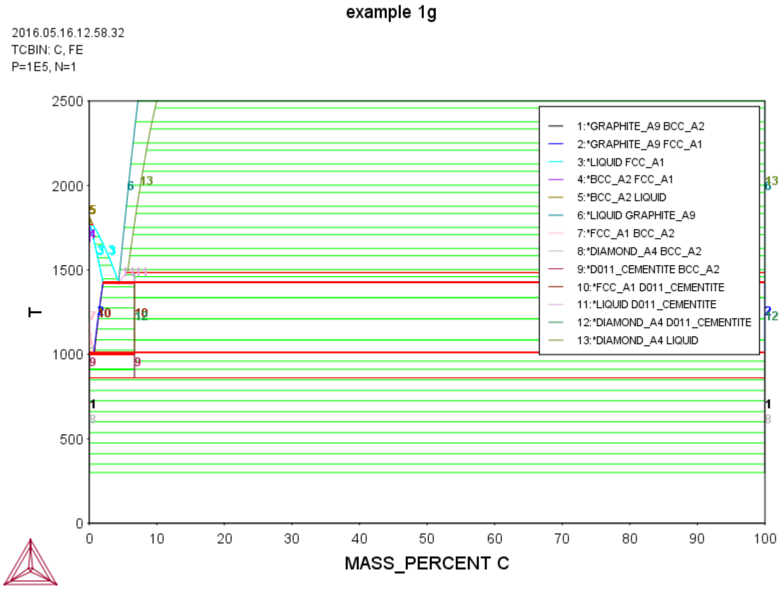
```
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28
Generating start point  29
Generating start point  30
Working hard
Generating start point  31
Generating start point  32

Phase region boundary   1 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary   2 at:   5.000E-01  3.000E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                     24  equilibria

Phase region boundary   3 at:   4.999E-01  8.605E+02
    BCC_A2
 ** D011_CEMENTITE
 ** DIAMOND_A4

Phase region boundary   4 at:   8.749E-01  8.605E+02
    BCC_A2
 ** D011_CEMENTITE
Calculated.                      7  equilibria

Phase region boundary   5 at:   8.746E-01  9.998E+02
    BCC_A2
 ** D011_CEMENTITE
 ** FCC_A1

Phase region boundary   6 at:   9.823E-01  9.998E+02
    BCC_A2
 ** FCC_A1
Calculated                     23  equilibria

Phase region boundary   7 at:   8.578E-01  9.998E+02
    D011_CEMENTITE
 ** FCC_A1
Calculated.                     18  equilibria

Phase region boundary   8 at:   8.354E-01  1.422E+03
 ** LIQUID
    D011_CEMENTITE
 ** FCC_A1

Phase region boundary   9 at:   7.872E-01  1.422E+03
 ** LIQUID
    D011_CEMENTITE
Calculated.                      5  equilibria

Phase region boundary  10 at:   7.657E-01  1.484E+03
 ** LIQUID
    D011_CEMENTITE
 ** DIAMOND_A4

Phase region boundary  11 at:   3.750E-01  1.484E+03
    D011_CEMENTITE
 ** DIAMOND_A4
Calculated.                     26  equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   3.907E-01  1.484E+03
    LIQUID
 ** DIAMOND_A4
Calculated..                     42  equilibria
Terminating at axis limit.

Phase region boundary  13 at:   8.678E-01  1.422E+03
 ** LIQUID
    FCC_A1
Calculated.                     15  equilibria

Phase region boundary  14 at:   9.840E-01  1.768E+03
 ** LIQUID
 ** BCC_A2
    FCC_A1

Phase region boundary  15 at:   9.939E-01  1.768E+03
 ** BCC_A2
    FCC_A1
Calculated                     25  equilibria

Phase region boundary  16 at:   9.858E-01  1.768E+03
    LIQUID
 ** BCC_A2
Calculated                     20  equilibria

Phase region boundary  17 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                     24  equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2  equilibria
```

```
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  19 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                     24  equilibria
Terminating at known equilibrium

Phase region boundary  20 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  21 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                     24  equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  23 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                     24  equilibria
Terminating at known equilibrium

Phase region boundary  24 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  25 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                     24  equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  27 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                     24  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   3.750E-01  1.037E+03
 ** D011_CEMENTITE
    DIAMOND_A4
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   3.750E-01  1.037E+03
 ** D011_CEMENTITE
    DIAMOND_A4
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   9.877E-01  1.037E+03
    BCC_A2
 ** FCC_A1
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   9.877E-01  1.037E+03
    BCC_A2
 ** FCC_A1
Calculated                     23  equilibria

Phase region boundary  32 at:   3.754E-01  1.763E+03
    LIQUID
 ** DIAMOND_A4
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   3.754E-01  1.763E+03
    LIQUID
 ** DIAMOND_A4
Calculated..                     31  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  34 at:   9.820E-01  1.763E+03
    LIQUID
 ** FCC_A1
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   9.820E-01  1.763E+03
    LIQUID
 ** FCC_A1
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  36 at:   3.306E-01  2.490E+03
    LIQUID
 ** DIAMOND_A4
Calculated.                     42  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   3.306E-01  2.490E+03
```

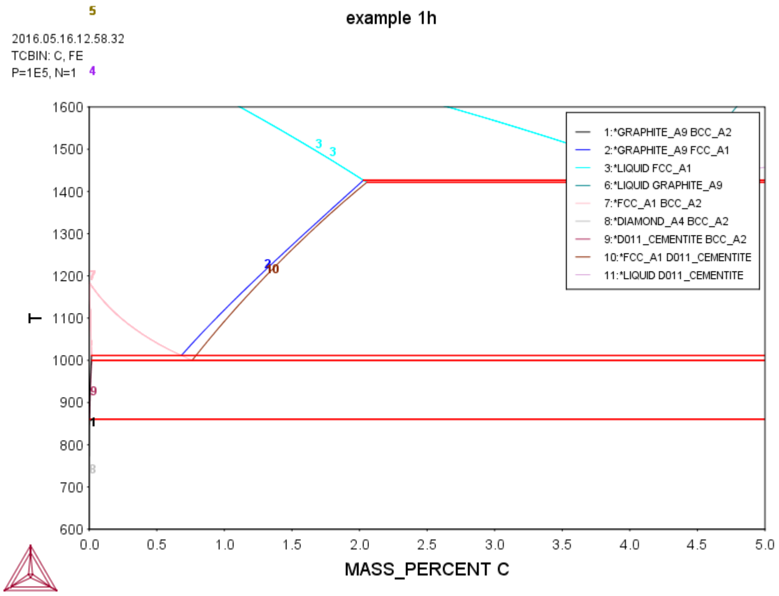
```
    LIQUID
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  38 at:   3.306E-01  2.490E+03
    LIQUID
 ** DIAMOND_A4
Calculated.                     42  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   3.306E-01  2.490E+03
    LIQUID
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  40 at:   3.306E-01  2.490E+03
    LIQUID
 ** DIAMOND_A4
Calculated.                     42  equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   3.306E-01  2.490E+03
    LIQUID
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  42 at:   3.317E-01  2.475E+03
    LIQUID
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  43 at:   3.317E-01  2.475E+03
    LIQUID
 ** DIAMOND_A4
Calculated.                     41  equilibria
Terminating at known equilibrium

Phase region boundary  44 at:   3.306E-01  2.490E+03
    LIQUID
 ** DIAMOND_A4
Calculated.                     42  equilibria
Terminating at known equilibrium

Phase region boundary  45 at:   3.306E-01  2.490E+03
    LIQUID
 ** DIAMOND_A4
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  46 at:   9.941E-01  1.794E+03
    LIQUID
 ** BCC_A2
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  47 at:   9.941E-01  1.794E+03
    LIQUID
 ** BCC_A2
Calculated                     12  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex01\BINA
RY.POLY3
CPU time for mapping                      1  seconds
POLY_3:
POLY_3: post
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x m-f C
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-tieline
   ... the command in full is SET_TIELINE_STATUS
PLOTTING EVERY TIE-LINE NO /5/: 5
POST:
POST: set-title example 1f
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



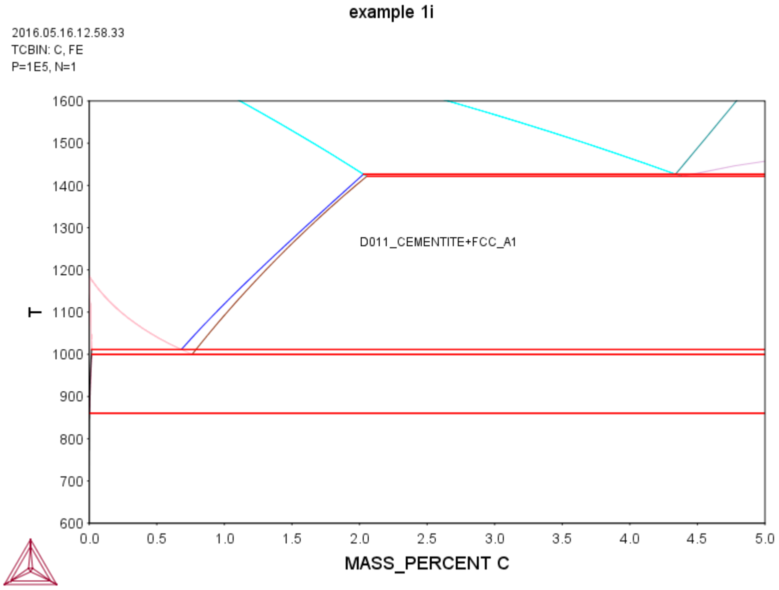
```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ The previous stable diagram is also plotted. The reason is that
POST: @@ we never removed it from the workspace (It can be done with a SAVE
POST: @@ command, please read about this command).
POST: @@
POST: @@ It may be surprising to find that diamond is more stable than
POST: @@ cementite at low temperature. However, one would never find
POST: @@ diamonds in steel, unfortunately, as graphite would form first.
POST: @@
POST: @@ Now change the axis to composition, use weight-percent of carbon
POST: s-d-a x
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
 UNKNOWN QUESTION VARIABLE :
VARIABLE : w-p
FOR COMPONENT : c
POST: set-title example 1g
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ The tie-lines now obscure the diagram, take them away
POST: @@ Also change the scale of the x and y axis
POST: s-t-s 0
   ... the command in full is SET_TIELINE_STATUS
POST: s-s x n 0 5
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 600 1600
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 1h
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

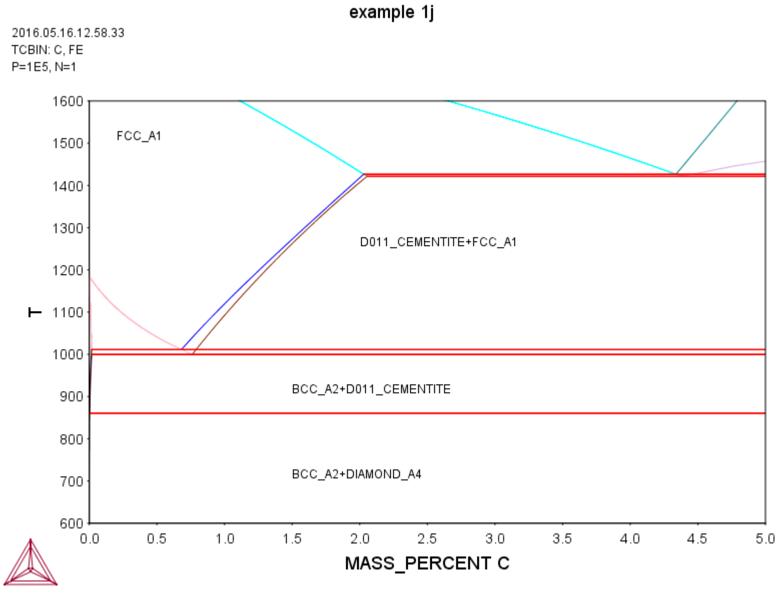


```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Finally add some nice labels
POST: set-lab n
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: add 2 1250
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated           413 grid points in               0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: D011_CEMENTITE+FCC_A1
Text size: /.36/:
POST: set-title example 1i
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

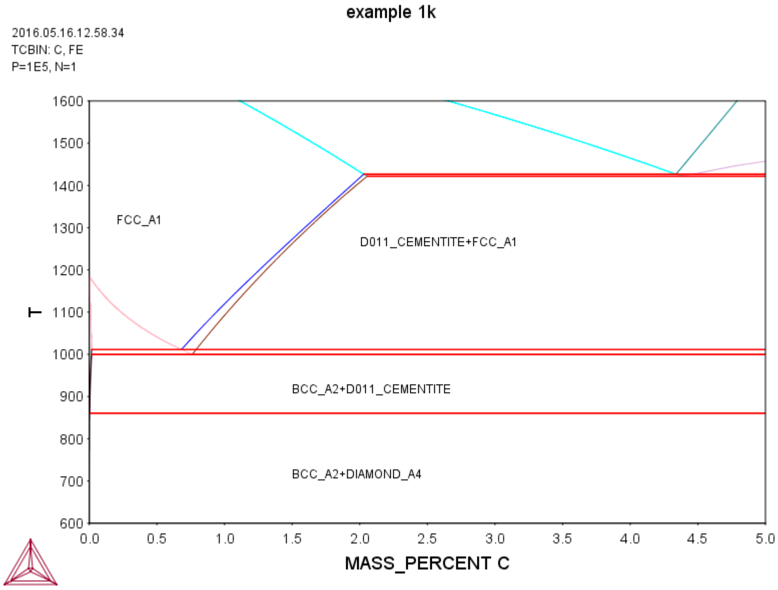


```
POST:
POST:
POST:Hit RETURN to continue
POST: add 1.5 900
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated           413 grid points in               0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: BCC_A2+D011_CEMENTITE
Text size: /.36/:
POST: add 1.5 700
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated           413 grid points in               0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: BCC_A2+DIAMOND_A4
Text size: /.36/:
POST: add .2 1500
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
```

```
Calculated           413 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: FCC_A1
Text size: /.36/:
POST: set-title example 1j
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ As graphite is suspended cementite is the stable carbide
POST: @@ so that is the phase that will be listed in the two-phase regions.
POST: @@ The label for the FCC region is a bit too high, move it down
POST: modify
   ... the command in full is MODIFY_LABEL_TEXT
 These labels are defined
 No    1 at  2.00000E+00 1.25000E+03 : D011_CEMENTITE+FCC_A1
 No    2 at  1.50000E+00 9.00000E+02 : BCC_A2+D011_CEMENTITE
 No    3 at  1.50000E+00 7.00000E+02 : BCC_A2+DIAMOND_A4
 No    4 at  2.00000E-01 1.50000E+03 : FCC_A1

Which label to modify? /4/:
New X coordinate /.2/: .2
New Y coordinate /1500/: 1300
New text /FCC_A1/:
POST: set-title example 1k
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

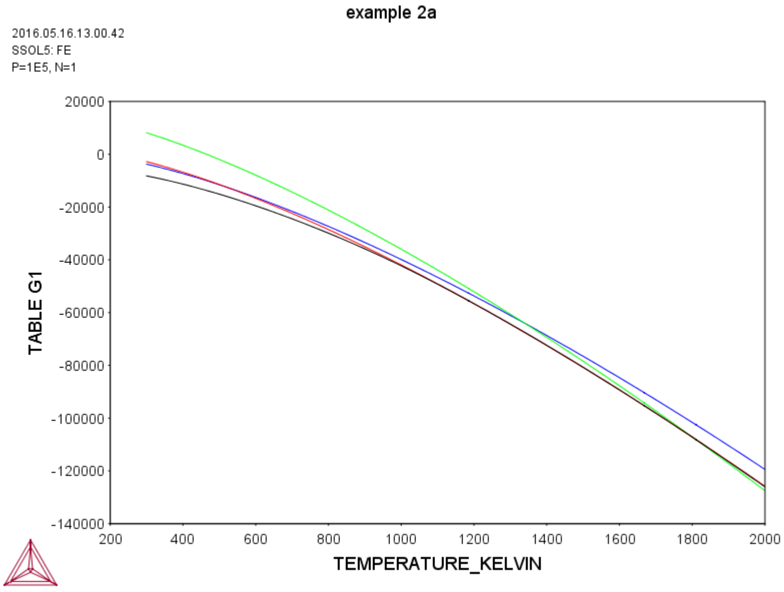


```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex02

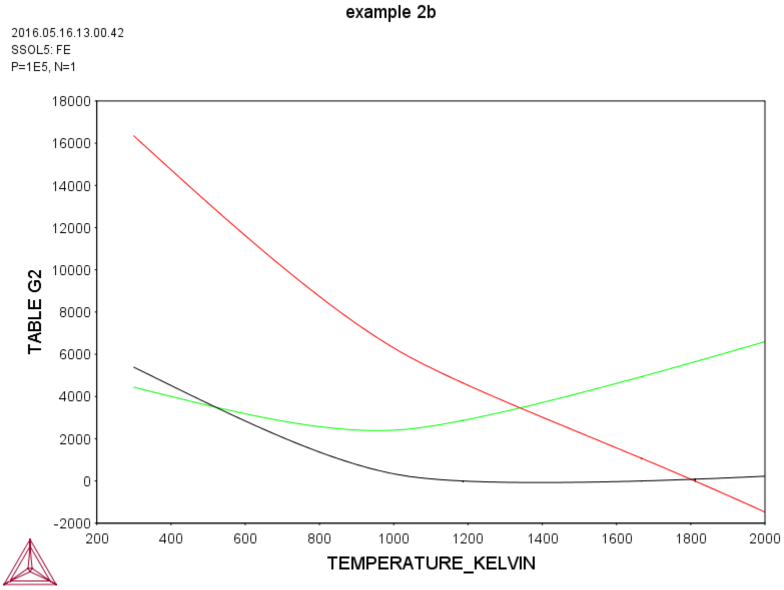
```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex02\tcex02.TCM"SYS:SYS:SYS:SYS:SYS:
SYS:
SYS:SYS:SYS: SET-ECHO
SYS: set-log ex02,,
SYS:
SYS:
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw ssol5
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Alloy Solutions Database v5.0

 VA  DEFINED
 GAS:G  REJECTED
TDB_SSOL5: @@ Pure Fe is selected as unary system
TDB_SSOL5: d-sys fe
   ... the command in full is DEFINE_SYSTEM
 FE  DEFINED
TDB_SSOL5: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Benyan Pei, B Bjorkman, B Sundman, and B Jansson: Calphad, 1995, 19(1), 1
      -15. "A thermodynamic assessment of the Iron-Antimony system". >> Fe
      -Sb '
  'G Reumont, P Perrot, JM Fiorani, and J Hertz: J. Phase Equil.,, 2000, 21,
      371-378. "Thermodynamic assessment of the Fe-Zn system". >> Fe-Zn '
 -OK-
TDB_SSOL5:
TDB_SSOL5: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ In POLY-3 we first define a single equilibrium
POLY_3: s-c t=300,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated            24 grid points in             0 s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL5

 Conditions:
 T=300, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    300.00 K (    26.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.58470E+01
 Total Gibbs energy -8.18407E+03,  Enthalpy  4.59751E+01,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 FE                      1.0000E+00  1.0000E+00 3.7589E-02 -8.1841E+03 SER

 BCC_B2                   DISORD Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.5847E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  1.00000E+00
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ We set T as axis variable
POLY_3: s-a-v
   ... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: t
Min value /0/: 300
Max value /1/: 2000
Increment /42.5/: 42.5
POLY_3: @@ We always save in order to be able to come back to this point
POLY_3: save tcex02a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ Step along the axis
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
 No initial equilibrium, using default
 Step will start from axis value    300.000
...OK

 Phase Region from    300.000     for:
     BCC_B2
 Global test at  3.80000E+02 .... OK
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
```

```
 Global test at  9.80000E+02 .... OK
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
 Global check of adding phase at  1.18481E+03
 Calculated    91 equilibria

 Phase Region from    1184.81     for:
     BCC_B2
     FCC_L12
 Calculated     2 equilibria

 Phase Region from    1184.81     for:
     FCC_L12
 Global test at  1.26000E+03 .... OK
 Global test at  1.36000E+03 .... OK
 Global test at  1.46000E+03 .... OK
 Global test at  1.56000E+03 .... OK
 Global test at  1.66000E+03 .... OK
 Global check of adding phase at  1.66747E+03
 Calculated    51 equilibria

 Phase Region from    1667.47     for:
     BCC_B2
     FCC_L12
 Calculated     2 equilibria

 Phase Region from    1667.47     for:
     BCC_B2
 Global test at  1.74000E+03 .... OK
 Global check of adding phase at  1.81095E+03
 Calculated    18 equilibria

 Phase Region from    1810.95     for:
     LIQUID
     BCC_B2
 Calculated     2 equilibria

 Phase Region from    1810.95     for:
     LIQUID
 Global test at  1.89000E+03 .... OK
 Global test at  1.99000E+03 .... OK
 Terminating at    2000.00
 Calculated    22 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex02\tcex
 02a.POLY3
POLY_3: @@ Post processing is the essential part of this example
POLY_3: @@ We will plot Gm, Hm and Cp for some phases
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: @@ The  x-axis will be the temperature in Kelvin
POST: s-d-a x
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
 UNKNOWN QUESTION VARIABLE :
VARIABLE : t-k
POST: @@ The phases for which Gm shall be plotted must be defined
POST: @@ in a table
POST: ent tab
   ... the command in full is ENTER_SYMBOL
Name: g1
Variable(s): gm(bcc_b2) gm(fcc_l12) gm(liq) gm(hcp_a3)
&
POST:
POST: @@ The table is set as y-axis and all columns included
POST: s-d-a y g1
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

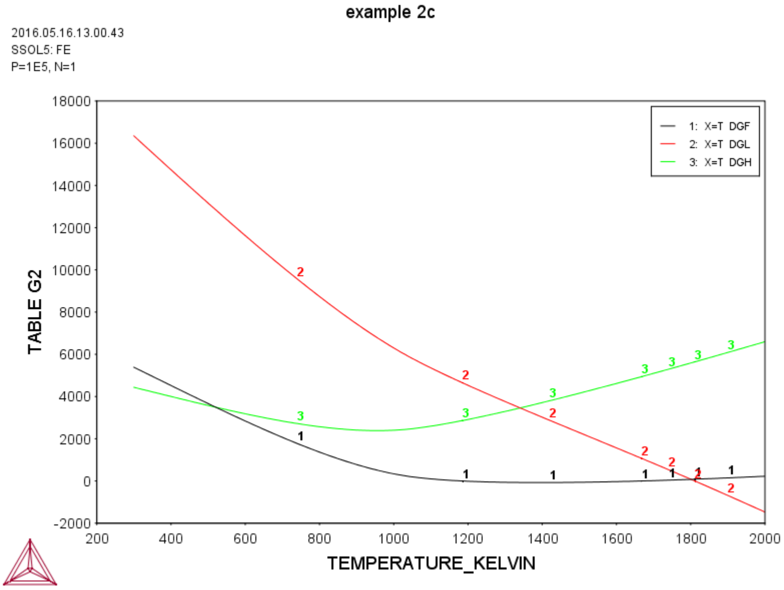


```
POST:
POST:Hit RETURN to continue
POST: @@
```

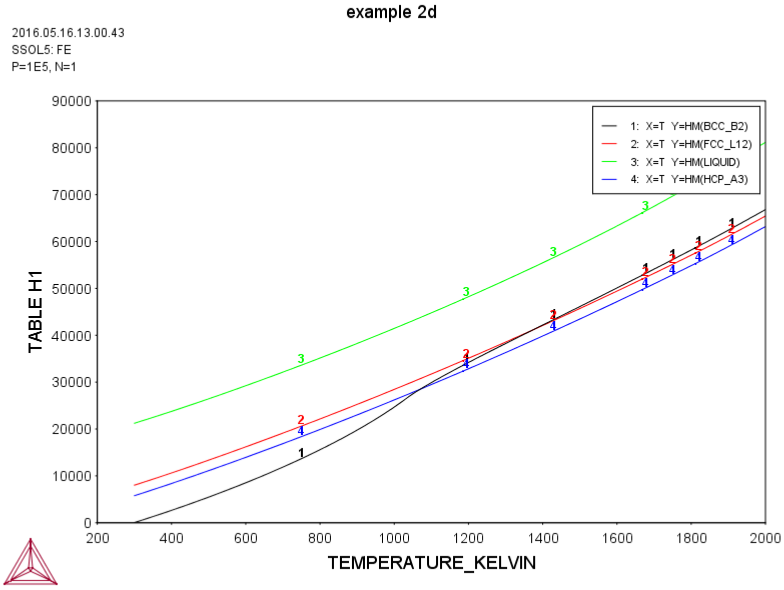
```
POST:
POST:
POST: @@ The magnitude makes it difficult to see anything. Enter
POST: @@ functions for the differences with respect to bcc
POST: ent fun dgf=gm(fcc_l12)-gm(bcc_b2);
   ... the command in full is ENTER_SYMBOL
POST: ent fun dgl=gm(liq)-gm(bcc_b2);
   ... the command in full is ENTER_SYMBOL
POST: ent fun dgh=gm(hcp_a3)-gm(bcc_b2);
   ... the command in full is ENTER_SYMBOL
POST: @@ and enter a new table and set it as y-axis
POST: ent tab g2
   ... the command in full is ENTER_SYMBOL
Variable(s): dgf dgl dgh;
POST: s-d-a y g2
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



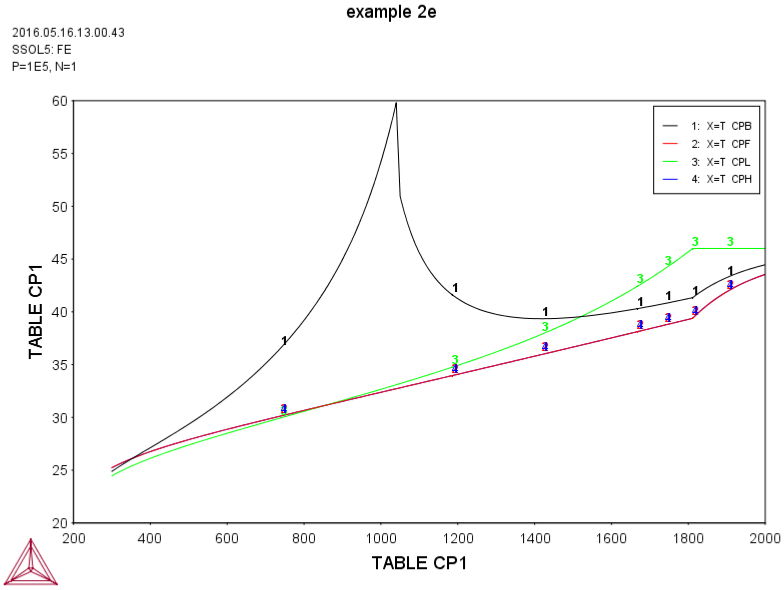
```
POST:
POST:Hit RETURN to continue
POST: @@ In order to have some identification on the lines
POST: @@ use the command SET_LABEL
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: D
POST: set-title example 2c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot enthalpies
POST: ent tab h1
   ... the command in full is ENTER_SYMBOL
Variable(s): hm(bcc_b2) hm(fcc_l12) hm(liq) hm(hcp_a3);
POST: s-d-a y h1
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



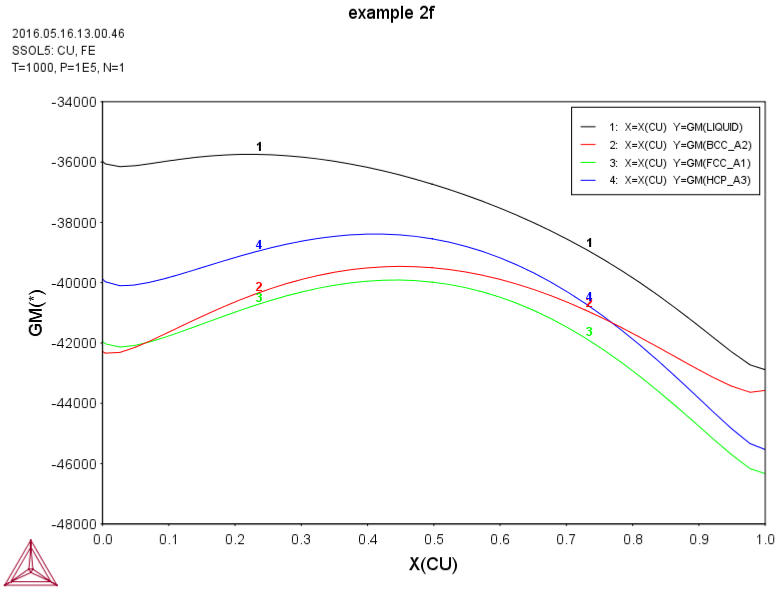
```
POST:
POST:Hit RETURN to continue
POST: @@ And finally plot heat capacities
POST: ent fun cpb=hm(bcc_b2).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cpf=hm(fcc_l12).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cpl=hm(liq).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cph=hm(hcp_a3).t;
   ... the command in full is ENTER_SYMBOL
POST: ent tab cp1
   ... the command in full is ENTER_SYMBOL
Variable(s): t cpb cpf cpl cph;
POST: s-d-a y
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : cp1
COLUMN NUMBER /*/: 2-5
POST: s-d-a x cp1 1
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 2e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



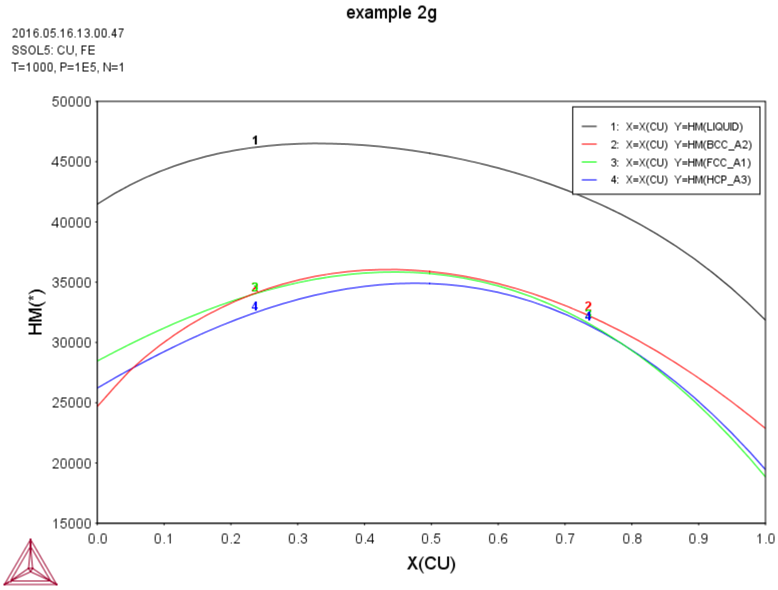
```
POST:
POST:Hit RETURN to continue
POST: @@
POST: @@ In the next case plot functions for a binary system
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: go da
   ... the command in full is GOTO_MODULE
TDB_SSOL5: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 GAS:G  REJECTED
 REINITIATING GES5 .....
TDB_SSOL5: @@ select the Cu-Fe system and only
TDB_SSOL5: @@ the fcc, bcc, liquid and hcp phases
TDB_SSOL5: d-sys fe cu
   ... the command in full is DEFINE_SYSTEM
 FE                      CU   DEFINED
TDB_SSOL5: rej ph /all
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  FCC_L12
 FCC_DIS                 FCC_ORD                 BCC_A2
 BCC_B2                  HCP_A3                  HCP_ZN
```

```
 TETRAGONAL_U            CBCC_A12                CUB_A13
 ORTHORHOMBIC_A20        LAVES_C14               LAVES_C15
 LAVES_C36               M4N                     ALCU_ETA
 ALCU_EPSILON            ALCUZN_GAMMA_H          AL5FE4
 CUSN_GAMMA_DO3          CUTI                    CU4TI
 CU6Y                    CUZN_GAMMA              D_GAMMA
 FEPD                    FEPD3                   FESB
 FEU6                    FE2U                    FEZN_GAMMA_D82
 FEZN4                   FEZN_DELTA              FEZN_ZETA
 FEUZR_DELTA             FEZR2                   FEZR3
   REJECTED
TDB_SSOL5: rest ph fcc_a1 bcc_a2 liq hcp_a3
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  LIQUID:L
 HCP_A3  RESTORED
TDB_SSOL5: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 LIQUID:L    :CU FE:
 FCC_A1      :CU FE:VA:
 BCC_A2      :CU FE:VA:
 HCP_A3      :CU FE:VA:
TDB_SSOL5: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Data for the Cu-Fe system are from an unpublished assessment of I Ansara
      and A Jansson published in the COST507 final report: COST507
      Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,
       AT Dinsdale and MH Rand, July 1998, EUR18499. The data were also
      reported by A Jansson in the KTH report TRITA-MAC-533, 1993. >> Cu-Fe '
 -OK-
TDB_SSOL5: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ set conditions for a single equilibrium
POLY_3: s-c t=1000,p=1e5,n=1,w(cu)=.01
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           548 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ select the fraction of Cu as axis variable
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(cu)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: @@ Save always
POLY_3: save tcex02b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ Now a special STEP option will be selected as the NORMAL
POLY_3: @@ option would only calculate the stable phases. The option
POLY_3: @@ SEPARATE means that all entered phases will be calculated
POLY_3: @@ separately.
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: ?
 The following options are available:
 NORMAL             Stepping with given conditions
 INITIAL_EQUILIBRIA An initial equilibrium stored at every step
 EVALUATE           Specified variables evaluated after each step
 SEPARATE_PHASES    Each phase calculated separately
 T-ZERO             T0 line calculation
 PARAEQUILIBRIUM    Paraequilibrium diagram
 MIXED_SCHEIL       Scheil with fast diffusing elements
 ONE_PHASE_AT_TIME  One phase at a time
Option? /NORMAL/: sep

 Phase Region from   0.529789     for:
     LIQUID
     BCC_A2
     FCC_A1
     HCP_A3

 Phase Region from   0.529789     for:
     LIQUID
     BCC_A2
     FCC_A1
     HCP_A3
 *** Buffer saved on file ***
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex02\tcex
 02b.POLY3
POLY_3: @@ Now plot the results in various ways
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: @@ Set the Gm of all phases on the y-axis
POST: s-d-a y gm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: @@ and the mole percent of Cu on the x-axis
POST: s-d-a x x(cu)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 2f
POST:
```

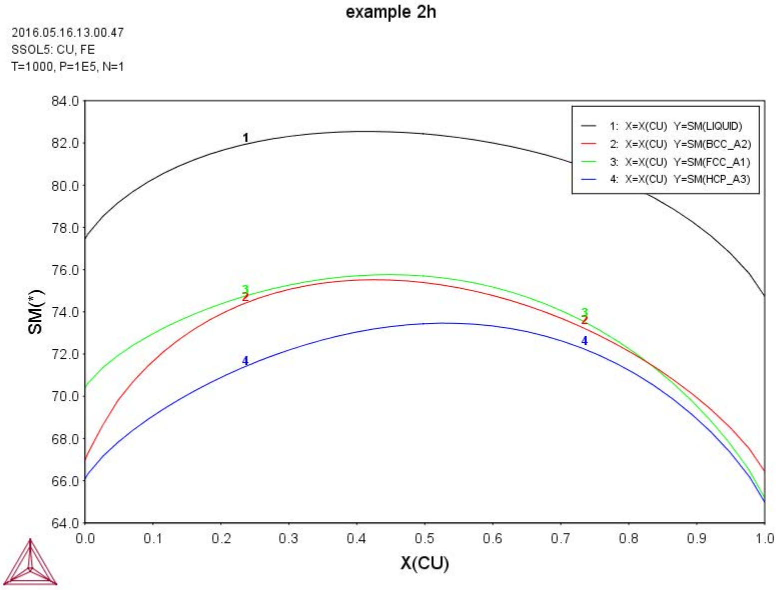
```
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot the enthalpy
POST: s-d-a y hm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2g
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



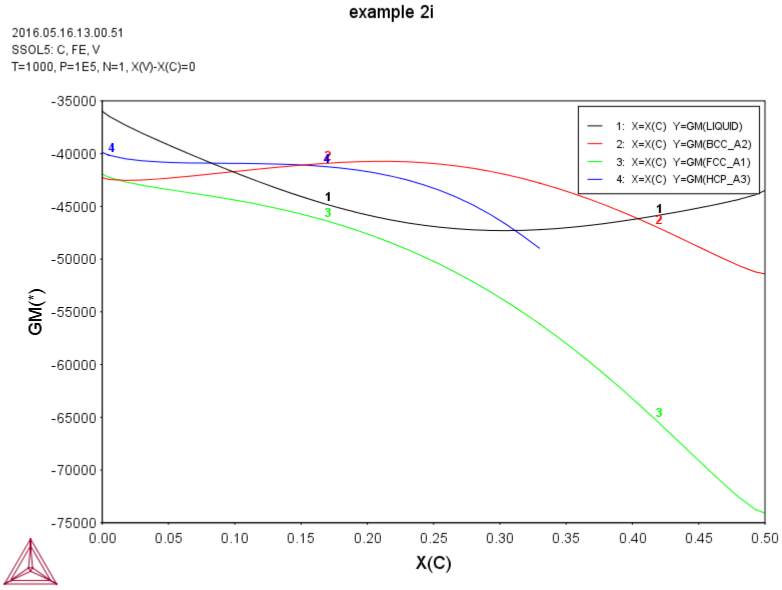
```
POST:
POST:Hit RETURN to continue
POST: @@ and finally the entropy
POST: s-d-a y sm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2h
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ The third case: ternary system, Fe-V-C
POST: @@ Calculate and plot Gm from the iron corner to VC
POST: ba
   ... the command in full is BACK
POLY_3: go da
   ... the command in full is GOTO_MODULE
TDB_SSOL5: rej sys
   ... the command in full is REJECT
 VA   DEFINED
 GAS:G   REJECTED
 REINITIATING GES5 .....
TDB_SSOL5: d-sys fe v c
   ... the command in full is DEFINE_SYSTEM
 FE                      V                       C
   DEFINED
TDB_SSOL5: rej ph / all
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  FCC_L12
 FCC_DIS                 FCC_ORD                 BCC_A2
 BCC_B2                  HCP_A3                  HCP_DIS
 HCP_ORD                 DIAMOND_A4              TETRAGONAL_U
 CBCC_A12                CUB_A13                 ORTHORHOMBIC_A20
 SIGMA                   GRAPHITE                LAVES_C14
 LAVES_C15               LAVES_C36               CEMENTITE
 KSI_CARBIDE             M23C6                   M7C3
 M3C2                    V3C2                    M5C2
 MC_ETA                  M4N                     FECN_CHI
 ALM_D019                AL5FE4                  ALTA_SIGMA
 ALTI                    FEPD                    FEPD3
 FESB                    FEU6                    FE2U
 FEZN_GAMMA_D82          FEZN4                   FEZN_DELTA
 FEZN_ZETA               FEUZR_DELTA             FEZR2
 FEZR3                   V3SI  REJECTED
TDB_SSOL5: rest ph fcc_a1 bcc_a2 hcp_a3 liq
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  HCP_A3
 LIQUID:L  RESTORED
TDB_SSOL5: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Data for the C-Fe system are taken from the assessment of P Gustafson,
      Report TRITA-MAC-0237, October 1984, Scand. J. Metall., 1985, 14, 259
      -267. Data for other phases not stable in the binary system are from:
      WM Huang: Report TRITA-MAC 411 (Rev 1989); Metall. Trans. A, 1990, 21A,
       2115-2123. WM Huang: Report TRITA-MAC 441 (1990), Metall. Trans. A,
      1991, 22A(9), 1911-1920. BJ Lee (1991), unpublished revision of data
      for C-Cr-Fe-Ni H Du and M Hillert: Z. Metallkde, 1991, 82(4), 310-316.
      H Du: J. Phase Equil., 1993, 14(6), 682-693. Note: Data for the V3C2
      phase were modified to be 10 J/mol more positive than those for the
      M3C2 phase. The data for the liquid data were modified by Tatjana
      Buhler to prevent bcc phase from becoming stable at high temperatures.
      >> C-Fe '
  'Data for the C-Fe-V system are taken the assessments of WM Huang: Report
      TRITA-MAC 432 (1990), Z. Metallkde, 1991, 82(5), 391-401. "A
      thermodynamic evaluation of the Fe-V-C system". BJ Lee and DN Lee:
      Report TRITA-MAC 474 (1991), Calphad, 1991, 15(3), 293-306. "A
      thermodynamic study on the Fe-V-C system". >> C-Fe-V '
  'Data for the C-V system are taken from the assessment of WM Huang: Z.
      Metallkde, 1991, 82, (3), 174-181. "An Assessment of the V-C System".
      Additional data are from further work by WM Huang: Report TRITA-MAC
      441 (1990), BJ Lee: Report TRITA-MAC 475 (1991). >> C-V '
  'Data for the Fe-V system are from the assessments of WM Huang: TRITA-MAC
      432 (Rev 1989,1990), Z. Metallkde, 1991, 82(5), 391-401. "A
      thermodynamic evaluation of the Fe-V-C system", WM Huang: Met. Trans.
      A, 1991, 22(9), 1911-1920. "Thermodynamic properties of the Fe-Mn-V-C
      system". >> Fe-V '
 -OK-
TDB_SSOL5: go p-3
```

```
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ set conditions for a single equilibrium
POLY_3: s-c t=1000,p=1e5,n=1,w(v)=.0015,x(c)=.001
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7434 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL5

 Conditions:
 T=1000, P=1E5, N=1, W(V)=1.5E-3, X(C)=1E-3
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.57951E+01
 Total Gibbs energy -4.23963E+04,  Enthalpy  2.45646E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        1.0000E-03  2.1527E-04 3.4515E-02 -2.7990E+04 SER
 FE                       9.9736E-01  9.9828E-01 6.1891E-03 -4.2279E+04 SER
 V                        1.6429E-03  1.5000E-03 4.0605E-07 -1.2236E+05 SER

 BCC_A2                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.9814E-01, Mass 5.5735E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.99368E-01  V   6.07213E-04  C   2.49276E-05

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.8638E-03, Mass 6.0520E-02, Volume fraction 0.0000E+00  Mass fractions:
 V   8.23694E-01  C   1.75507E-01  FE  7.99487E-04
POLY_3:Hit RETURN to continue
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    1.863776E-03
 BCC_A2                   ENTERED      0.000000E+00    9.981362E-01
 HCP_A3                   ENTERED     -2.875358E-01    0.000000E+00
 HCP_A3#2                 ENTERED     -2.875358E-01    0.000000E+00
 LIQUID                   ENTERED     -6.510578E-01    0.000000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Note we have several composition sets because fcc
POLY_3: @@ (and possibly hcp) can exist both as metallic and
POLY_3: @@ as carbide. However, in this case it is unecessary
POLY_3: @@ as we are only interested in the value of the
POLY_3: @@ thermodynamic functions, not the equilibrium, and therefore
POLY_3: @@ we suspend them
POLY_3:
POLY_3: c-s p hcp_a3#2
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: sus
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1000, P=1E5, N=1, W(V)=1.5E-3, X(C)=1E-3
 DEGREES OF FREEDOM 0
POLY_3: @@ We would like to calculate the Gibbs energy from
POLY_3: @@ pure Fe to the corner VC. Select a line with equal
POLY_3: @@ fraction of V and C
POLY_3: s-c x(v)-x(c)=0
   ... the command in full is SET_CONDITION
POLY_3: s-c w(v)=none
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1000, P=1E5, N=1, X(C)=1E-3, X(V)-X(C)=0
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          7434 grid points in             0 s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL5

 Conditions:
 T=1000, P=1E5, N=1, X(C)=1E-3, X(V)-X(C)=0
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.57983E+01
 Total Gibbs energy -4.23424E+04,  Enthalpy  2.46245E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        1.0000E-03  2.1526E-04 9.5381E-02 -1.9538E+04 SER
 FE                       9.9800E-01  9.9887E-01 6.1904E-03 -4.2277E+04 SER
 V                        1.0000E-03  9.1295E-04 1.6021E-07 -1.3010E+05 SER

 BCC_A2                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.9858E-01, Mass 5.5752E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.99691E-01  V   2.40126E-04  C   6.83917E-05

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.4208E-03, Mass 4.5810E-02, Volume fraction 0.0000E+00  Mass fractions:
 V   8.19759E-01  C   1.78955E-01  FE  1.28625E-03
POLY_3:Hit RETURN to continue
POLY_3: @@ Set the fraction of C as axis
POLY_3: @@ The fraction of V will be the same
POLY_3: s-a-v
   ... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: x(c)
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .0125
POLY_3: save tcex02c y
   ... the command in full is SAVE_WORKSPACES
```

```
POLY_3: @@ step along the axis
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: sep

 Phase Region from   0.330065     for:
     LIQUID
     BCC_A2
     FCC_A1

 Phase Region from   0.330065     for:
     LIQUID
     BCC_A2
     FCC_A1

 Phase Region from   0.480604E-02 for:
     HCP_A3

 Phase Region from   0.480604E-02 for:
     HCP_A3
 *** Buffer saved on file ***
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex02\tcex
 02c.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: @@ plot the Gm versus carbon content
POST: l-p-s
   ... the command in full is LIST_PLOT_SETTINGS
 GRAPHIC DEVICE: TC-UNITE Driver ( #22)  PLOTFILE: SCREEN
 FONT:   (# 1)  Arial Bold
 AXIS PLOT             YES
 RASTER PLOT          : NO
 TRIANGULAR PLOT      : NO

 AUTOMATIC SCALING

 AUTOMATIC AXIS TEXT

 AXIS VARIABLES
POST: s-d-a x x(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y gm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST:
POST: set-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 2i
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ The fourth case: more partial derivatives
POST: back
POLY_3: go da
   ... the command in full is GOTO_MODULE
TDB_SSOL5: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 GAS:G  REJECTED
 REINITIATING GES5 .....
TDB_SSOL5: def-sys al cu
   ... the command in full is DEFINE_SYSTEM
 AL                         CU  DEFINED
TDB_SSOL5: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
```

```
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Taken from ACMSZ-1, based on unpublished assessment of N Saunders
      published in the COST507 final report COST507 Thermochemical database
      for light metal alloys, Volume 2 eds I Ansara, A T Dinsdale and M H
      Rand, July 1998, EUR18499 Updates from V.T. Witusiewicz, U. Hecht,
      S.G. Fries, S. Rex, JALCOM 385 (2004) 133-143 (Al-Cu) and H.Liang,
      Y.A.Chang, JPE 19 (1998) 25-37 (Al-Cu-Zn). >> Al-Cu '
  'Data for the Al-Li system are from an unpublished assessment of N
      Saunders published in the COST507 final report: COST507 Thermochemical
      Database for Light Metal Alloys, Vol 2, eds by I Ansara, AT Dinsdale
      and MH Rand, July 1998, EUR18499. >> Al-Li '
  'C Servant and I Ansara: J. Chim. Phys. 1997, 94, 869-888. "Thermodynamic
      assessment of the Al-Nb system". >> Al-Nb '
  'B Sundman, SG Fries, and WA Oates: Calphad, 1998, 22(3), 335-354. "A
      Thermodynamic Assessment of the Au-Cu System - An example illustrating
      the need for more physics in Calphad Solution Models". Two different
      datasets are given in the paper. The adopted assessment was derived by
      considering the chemical ordering. >> Au-Cu '
  'SG Fries, HL Lukas, R Konetzki, and R Schmid-Fetzer: J. Phase Equil.,
      1994, 15(6), 606-614. "Experimental investigation and thermodynamic
      optimization of the Y-Cu binary system". Note: The data for the CuY
      phase have been modified slightly to correct the calculated invariant
      temperatures. >> Cu-Y '
  'M Kowalski and PJ Spencer: J. Phase Equil., 1993, 14(4), 432-438. "
      Thermodynamic reevaluation of the Cu-Zn system". Some v. minor
      differences in gamma_brass data wrt SOLDERS >> Cu-Zn '
 -OK-
TDB_SSOL5: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1400 p=1e5 n=1 x(al)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         13716 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL5

 Conditions:
 T=1400, P=1E5, N=1, X(AL)=0.1
 DEGREES OF FREEDOM 0

 Temperature   1400.00 K (  1126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.98896E+01
 Total Gibbs energy -8.53069E+04,  Enthalpy  3.62263E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      1.0000E-01  4.5053E-02 1.3593E-06 -1.5724E+05 SER
 CU                      9.0000E-01  9.5495E-01 1.3045E-03 -7.7314E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.9890E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  9.54947E-01  AL  4.50529E-02
POLY_3:Hit RETURN to continue
POLY_3: @@ check the activity of aluminum
POLY_3: show acr(al)
   ... the command in full is SHOW_VALUE
 ACR(AL)=1.359263E-6
POLY_3: @@ This activity value is referred to fcc Al at 298.15 K.
POLY_3: @@ Set proper reference state for activities
POLY_3: set-ref-state al
   ... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature /*/:
Pressure /1E5/:
POLY_3:
POLY_3: set-ref-state cu
   ... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature /*/:
Pressure /1E5/:
POLY_3:
POLY_3: show acr(al)
   ... the command in full is SHOW_VALUE
 ACR(AL)=8.0990275E-4
POLY_3: @@ This value is better.  The corresponding chemical potential is
POLY_3: show mur(al)
   ... the command in full is SHOW_VALUE
 MUR(AL)=-82862.697
POLY_3: @@ The relation is simply that acr(al)=exp(mur(al)/RT).  Check that
POLY_3: enter fun test
   ... the command in full is ENTER_SYMBOL
Function: exp(mur(al)/8.31451/T);
POLY_3: show test
   ... the command in full is SHOW_VALUE
 TEST=8.0990275E-4
POLY_3:Hit RETURN to continue
POLY_3: @@ POLY allows calculation of partial derivatives of thermodynamic
POLY_3: @@ quantities of original reference state with respect to fractions
POLY_3: @@ that are conditions. For example
POLY_3: show gm.x(al)
   ... the command in full is SHOW_VALUE
 GM.X(AL)=-79930.097
POLY_3: @@ This is not the same as the chemical potential. It actually
POLY_3: @@ equals to the so-called diffusion potential: mu(al)-mu(cu).
POLY_3: ent fun diffmu=mu(al)-mu(cu);
   ... the command in full is ENTER_SYMBOL
POLY_3: show diffmu
   ... the command in full is SHOW_VALUE
 DIFFMU=-79930.097
POLY_3: @@ The relation between the chemical potential and the partial derivative is
POLY_3: @@
```

```
POLY_3: @@ mu(al) = gm + gm.x(al) - x(al)*gm.x(al)
POLY_3: @@
POLY_3: @@ We can enter this as a function also.
POLY_3: enter fun dgdx=gm+gm.x(al)-x(al)*gm.x(al);
   ... the command in full is ENTER_SYMBOL
POLY_3: sh dgdx
   ... the command in full is SHOW_VALUE

 Warning: All functions are evaluated for this command and as there are
 one or more functions with a derivative which may be irrelevant
 for this equilibrium some functions may have wrong values.
 If possible enter derivatives as VARIABLES instead

 DGDX=-157243.97
POLY_3: sh mu(al)
   ... the command in full is SHOW_VALUE
 MU(AL)=-157243.97
POLY_3: @@ Partial entropy is the negative of mu(al).t
POLY_3: ent fun ps=-mu(al).t;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh ps
   ... the command in full is SHOW_VALUE

 Warning: All functions are evaluated for this command and as there are
 one or more functions with a derivative which may be irrelevant
 for this equilibrium some functions may have wrong values.
 If possible enter derivatives as VARIABLES instead

 PS=95.218667
POLY_3: @@ Partial enthalpy is h = g + s*t
POLY_3: enter fun ph=mu(al)+ps*t;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh ph
   ... the command in full is SHOW_VALUE

 Warning: All functions are evaluated for this command and as there are
 one or more functions with a derivative which may be irrelevant
 for this equilibrium some functions may have wrong values.
 If possible enter derivatives as VARIABLES instead

 PH=-23937.838
POLY_3: @@ Partial enthalpy can also be calculated in a similar way as chemical
POLY_3: @@ potential
POLY_3: @@ partial enthalpy = hm + hm.x(al) - x(al)*hm.x(al)
POLY_3: ent fun ph1=hm+hm.x(al)-x(al)*hm.x(al);
   ... the command in full is ENTER_SYMBOL
POLY_3: sh ph1
   ... the command in full is SHOW_VALUE

 Warning: All functions are evaluated for this command and as there are
 one or more functions with a derivative which may be irrelevant
 for this equilibrium some functions may have wrong values.
 If possible enter derivatives as VARIABLES instead

 PH1=-23937.838
POLY_3: @@ As can be seen, ph1 = ph.
POLY_3: @@ Another useful quantity is mu(al).x(al).  That is related to
POLY_3: @@ the thermodynamic factor and part of the diffusion coefficient.
POLY_3: show mu(al).x(al)
   ... the command in full is SHOW_VALUE
 MU(AL).X(AL)=324789.82
POLY_3:
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3:
```

tcex03

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex03\tcex03.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of an isothermal section using TERNARY module
SYS: @@
SYS: set-log ex03,,
SYS:
SYS: go tern
   ... the command in full is GOTO_MODULE

 Quick ternary phase diagram calculation module

 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 Current database: Iron Demo Database

 VA                      /-  DEFINED
Database: /FEDEMO/: FEDEMO
First element: ?
 The following assessed systems
   C-CR-FE  C-CR  C-FE  CR-FE

First element: fe
Second element: c
Third element: cr
Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/: Phase_Diagram
Temperature (C) /1000/: 1200
Global minimization on: /Y/:
 VA                      /-  DEFINED
 REINITIATING GES5 .....
 C                       CR                      FE
   DEFINED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
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      (1986); CR-FE'
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      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
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  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
      (1986); CR-FE-MO'
  'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, estimated parameter 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
 The condition X(CR)=.1234  created
 The condition X(FE)=.1234  created
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
```
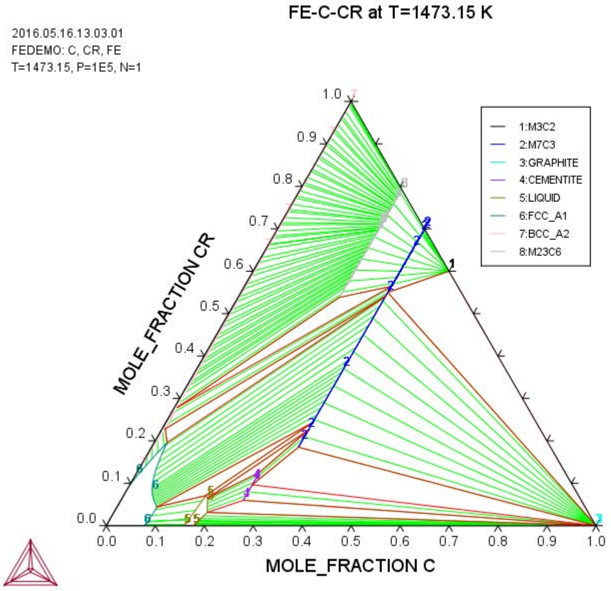
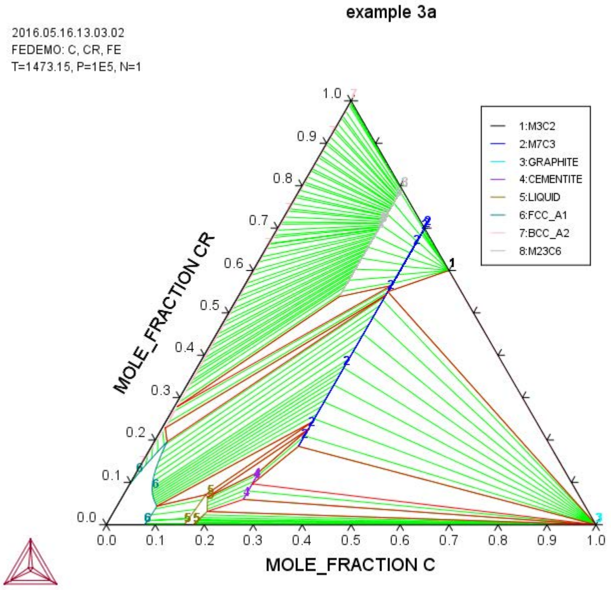

```
Working hard
Generating start point  11
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Generating start point  21

Phase region boundary   1 at:   1.750E-01  1.750E-01
 ** GRAPHITE
    M7C3
Calculated.                     11  equilibria

Phase region boundary   2 at:   2.749E-01  7.508E-02
 ** GRAPHITE
 ** M3C2
    M7C3

Phase region boundary   3 at:   5.749E-01  7.508E-02
 ** M3C2
    M7C3
Calculated                     18  equilibria

Phase region boundary   4 at:   3.000E-01  0.000E+00
    GRAPHITE
 ** M3C2

Phase region boundary   5 at:   2.749E-01  7.508E-02
 ** GRAPHITE
    M7C3
Calculated.                     20  equilibria

Phase region boundary   6 at:   9.248E-02  2.575E-01
 ** CEMENTITE
 ** GRAPHITE
    M7C3

Phase region boundary   7 at:   1.406E-01  5.844E-01
 ** CEMENTITE
    M7C3
Calculated.                      5  equilibria

Phase region boundary   8 at:   1.754E-01  5.496E-01
 ** LIQUID
 ** CEMENTITE
    M7C3

Phase region boundary   9 at:   1.452E-01  6.174E-01
 ** LIQUID
    M7C3
Calculated.                      3  equilibria

Phase region boundary  10 at:   1.571E-01  6.091E-01
 ** LIQUID
 ** FCC_A1#2
    M7C3

Phase region boundary  11 at:   1.436E-01  6.656E-01
 ** FCC_A1
    M7C3
Calculated.                     32  equilibria

Phase region boundary  12 at:   3.786E-01  4.505E-01
 ** BCC_A2
 ** FCC_A1
    M7C3

Phase region boundary  13 at:   3.849E-01  4.619E-01
 ** BCC_A2
    M7C3
Calculated.                      5  equilibria

Phase region boundary  14 at:   4.217E-01  4.253E-01
 ** BCC_A2
 ** M23C6
    M7C3

Phase region boundary  15 at:   5.511E-01  1.954E-01
 ** M23C6
    M7C3
Calculated                     30  equilibria

Phase region boundary  16 at:   4.085E-01  4.850E-01
    BCC_A2
 ** M23C6
Calculated                     56  equilibria

Phase region boundary  17 at:   2.122E-01  7.714E-01
 ** BCC_A2
    FCC_A1
Calculated                     24  equilibria

Phase region boundary  18 at:   5.747E-02  8.179E-01
    LIQUID
 ** FCC_A1
Calculated                     24  equilibria

Phase region boundary  19 at:   9.527E-02  6.924E-01
 ** LIQUID
    CEMENTITE
Calculated.                      9  equilibria

Phase region boundary  20 at:   4.556E-02  7.341E-01
 ** LIQUID
    CEMENTITE
 ** GRAPHITE

Phase region boundary  21 at:   2.996E-02  3.450E-01
    CEMENTITE
 ** GRAPHITE
Calculated.                      3  equilibria
```

```
Terminating at known equilibrium

Phase region boundary  22 at:   1.560E-02  3.890E-01
    LIQUID
 ** GRAPHITE
Calculated                     23  equilibria

Phase region boundary  23 at:   1.750E-01  1.750E-01
 ** GRAPHITE
    M7C3
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  24 at:   1.750E-01  1.750E-01
 ** GRAPHITE
    M7C3
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   1.750E-01  1.750E-01
 ** GRAPHITE
    M7C3
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   3.000E-01  0.000E+00
    GRAPHITE
 ** M3C2

Phase region boundary  27 at:   2.749E-01  7.508E-02
 ** GRAPHITE
    M7C3
Calculated.                     20  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   5.749E-01  7.508E-02
 ** M3C2
    M7C3
Calculated                     21  equilibria

Phase region boundary  29 at:   6.432E-01  6.818E-03
 ** M3C2
    M7C3
Calculated                     15  equilibria

Phase region boundary  30 at:   6.432E-01  6.818E-03
 ** M3C2
    M7C3
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   8.931E-01  3.310E-03
    BCC_A2
 ** M23C6
Calculated                     11  equilibria

Phase region boundary  32 at:   8.931E-01  3.310E-03
    BCC_A2
 ** M23C6
Calculated.                     50  equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   1.172E-02  3.945E-01
    LIQUID
 ** GRAPHITE
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   1.172E-02  3.945E-01
    LIQUID
 ** GRAPHITE
Calculated                     24  equilibria

Phase region boundary  35 at:   6.066E-03  4.024E-01
    LIQUID
 ** GRAPHITE
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  36 at:   6.066E-03  4.024E-01
    LIQUID
 ** GRAPHITE
Calculated                     19  equilibria

Phase region boundary  37 at:   1.253E-02  8.670E-01
 ** LIQUID
    FCC_A1
Calculated                     12  equilibria

Phase region boundary  38 at:   1.253E-02  8.670E-01
 ** LIQUID
    FCC_A1
Calculated.                      7  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   4.511E-01  4.428E-01
    BCC_A2
 ** M23C6
Calculated                     57  equilibria

Phase region boundary  40 at:   4.511E-01  4.428E-01
    BCC_A2
 ** M23C6
Calculated.                      6  equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   6.796E-01  2.160E-01
    BCC_A2
 ** M23C6
Calculated                     35  equilibria

Phase region boundary  42 at:   6.796E-01  2.160E-01
    BCC_A2
 ** M23C6
Calculated.                     28  equilibria
Terminating at known equilibrium
```

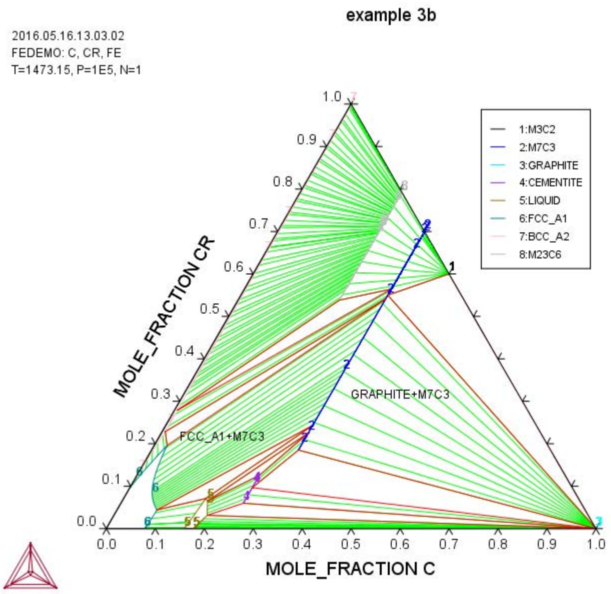
```
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex03\ISOT
 HER.POLY3
 CPU time for mapping                      3  seconds

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes


  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes
```



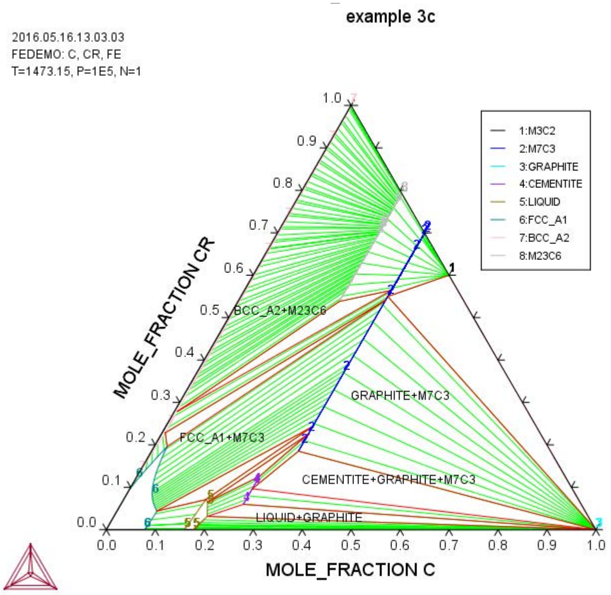
```
POST:
POST: set-title example 3a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



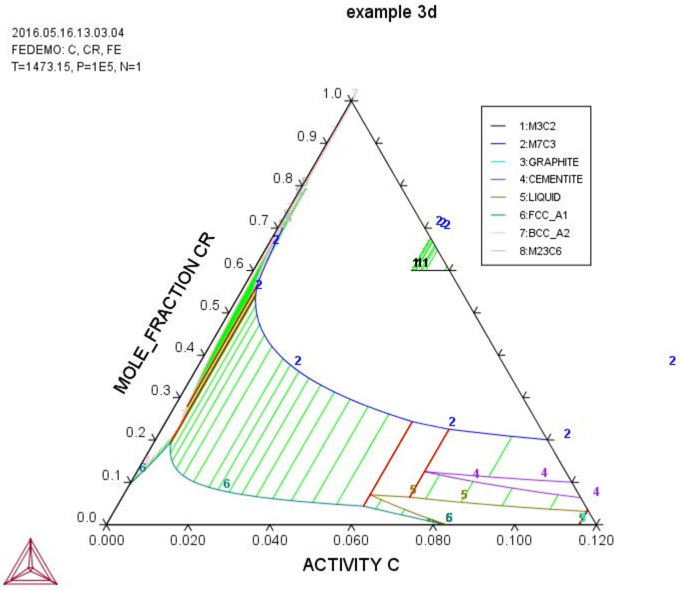
```
POST:
POST:Hit RETURN to continue
POST: @@ Add some labels
POST: add .35 .3
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: GRAPHITE+M7C3
Text size: /.36/:
POST: add .05 .2
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: FCC_A1+M7C3
Text size: /.36/:
POST: set-title example 3b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



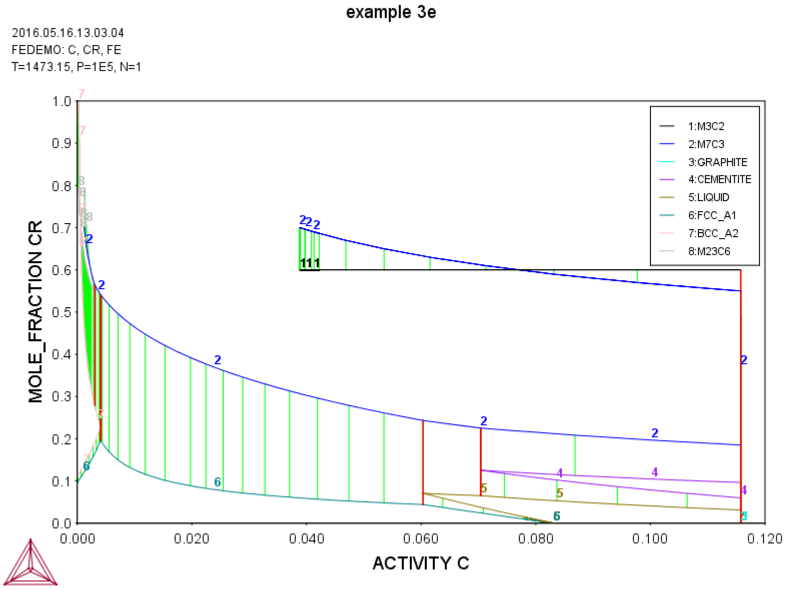
```
POST:
POST:Hit RETURN to continue
POST: add .3 .01
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: LIQUID+GRAPHITE
Text size: /.36/:
POST: add .35 .1
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in               0 s
 Calculated POLY solution       1 s, total time      1  s
 Stable phases are: CEMENTITE+GRAPHITE+M7C3
Text size: /.36/:
POST: add .01 .5
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: BCC_A2+M23C6
Text size: /.36/:
POST: set-title example 3c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



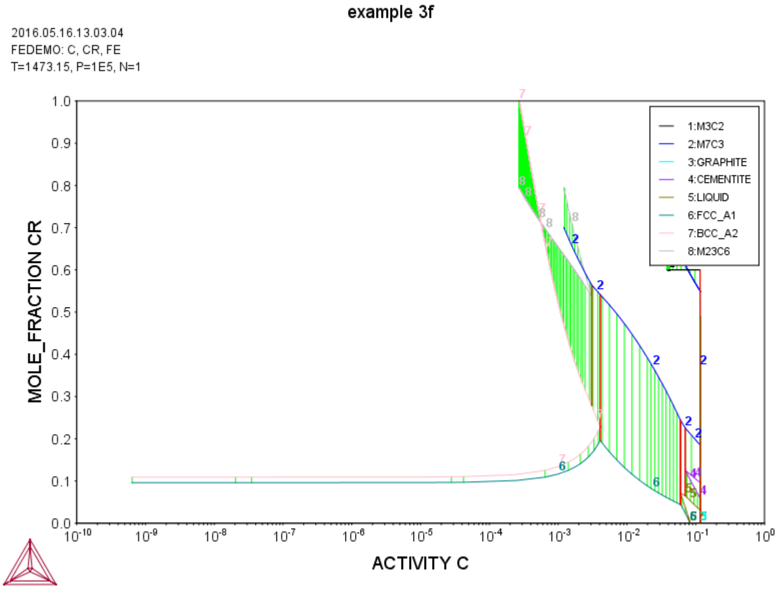
```
POST:
POST:Hit RETURN to continue
POST: @@ We can try the same exercise as in example 1, use
POST: @@ carbon activity as one axis
POST: s-d-a x ac c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 3d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ With these axes it is better to have a square diagram!
POST: s-dia-type
   ... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM  (Y OR N) /N/: N
CREATE TETRAHEDRON WRML FILE  (Y OR N) /N/:
POST:
POST: set-title example 3e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

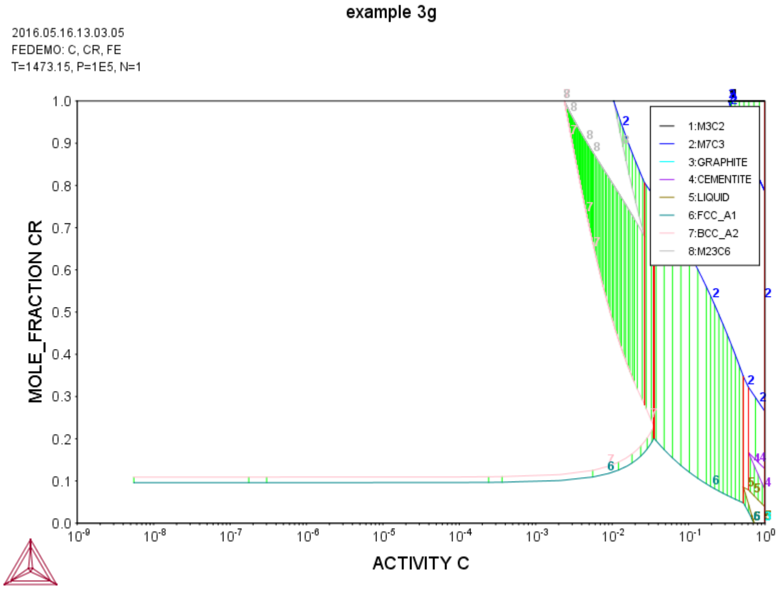


```
POST:
POST:Hit RETURN to continue
POST: @@ The activity axis is probably better as logarithmic
POST: s-a-ty x
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 3f
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

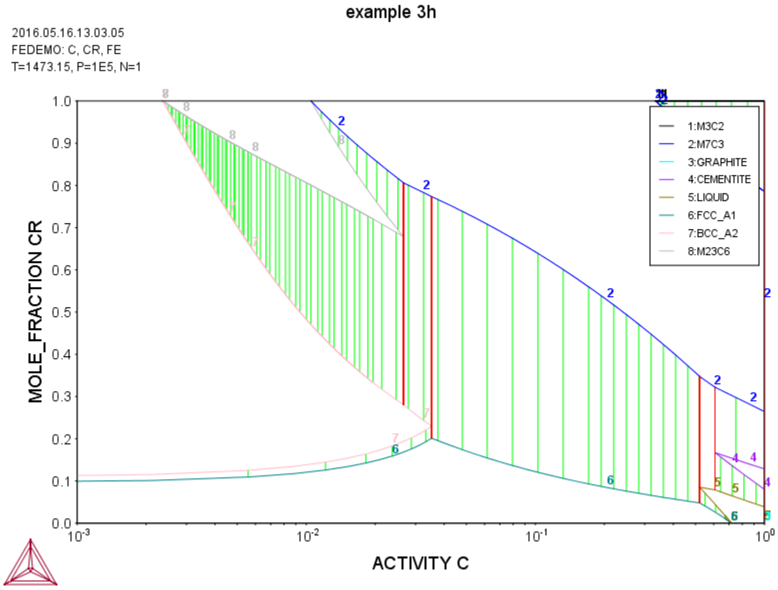


```
POST:
POST:Hit RETURN to continue
POST: @@ In order for pure graphite to have activity one, the reference
POST: @@ state of C should be set to graphite. In addition,
POST: @@ the solubility lines now cross! Is the diagram wrong?
POST: @@ No, in this case one should not use the mole fraction of Cr
POST: @@ but the metallic fraction. This can be set by setting
POST: @@ the status of C to "special". All species set as special
POST: @@ will be excluded from the summation of fractions.
POST: @@ The special status is set in the POLY module
POST: ba
   ... the command in full is BACK
SYS: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: s-r-s
   ... the command in full is SET_REFERENCE_STATE
Component: c
Reference phase: gra
Temperature /*/:
Pressure /1E5/:
POLY_3: ch-st
   ... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/: c
Name(s): c
Status: /ENTERED/: ?

 Status

  The new status to be assigned must be given.

   * For species, the values ENTERED or SUSPENDED can be used.

   * For components, the status ENTERED, SUSPENDED or SPECIAL can be given.
       SPECIAL means that this component will be excluded from sums for
       mole fractions and mass fractions.

   * For phases, the status ENTERED, SUSPENDED, DORMANT or FIXED can be given.
       DORMANT means the same as suspended but the driving force will be
       calculated. FIXED means that it is a condition that the phase is
       stable at a certain amount.

  Note that only component(s) may have the status SPECIAL, which implies
   that they will not be included in summations for mole or mass fractions.
   For instance, for the so-called "u" fractions or other normalized fractions,
   when one or more of the components are excluded from the summation, one
   must specify which component(s) should be excluded from the calculation
   of mole or mass fraction. This component status is particularly useful
   when calculating paraequilibrium states. Such component(s) are normally
   interstitial component, and must have the status SPECIAL. This is assigned
   by the CHANGE_STATUS command. For example, to obtain the metallic fraction
   in a system with as an intersitial component, one can set the component
   status for carbon as SPECIAL:
     Change_status comp C=special

  Important Note: Special attentions should be paid when specifying a FIXED
   phase status in equilibrium calculations (for single points, stepping or
   mapping calculations), as described below:

   * The phase amount variables, NP(phase), BP(phase) and VP(phase), as well
     as all their M/W/V-suffixed quantities, should not be used as conditions.
     Instead, one can use the CHANGE_STATUS command to set a relevant
     condition, e.g., CHANGE_STATUS phase <phase>=fix <amount> where the
     fixed <amount> is roughly the same as the F-suffixed quantity "NPF(phase)".

   * The "NPF(phase)" quantity is the normalized mole number of components
     (per mole formula unit) of the specific phase in the defined system,
     which unlike other F-suffixed state variables [e.g., GF(phase),
     HF(phase) and DGF(phase)] can not be directly applied in any POLY
     command, implying that it can not be directly evaluated or listed/shown.
     If intended to shown such a normalized phase amount value in an
     equilibrium state, one should instead use a properly-entered symbol
     (function or variable), for instance,
           NPFabc = NP(abc)/NA
       or  NPFabc = NPM(abc)/NA*N
     N is the total system size (in mole). The NA value is a quantity that
     is phase-dependent (and sometimes also equilibrium-dependent for ionic
     solution phases), and is the total atomic number in a mole-formula-unit
     of the specific phase abc (excluding interstitial component and, of
     course, vacancy).
```

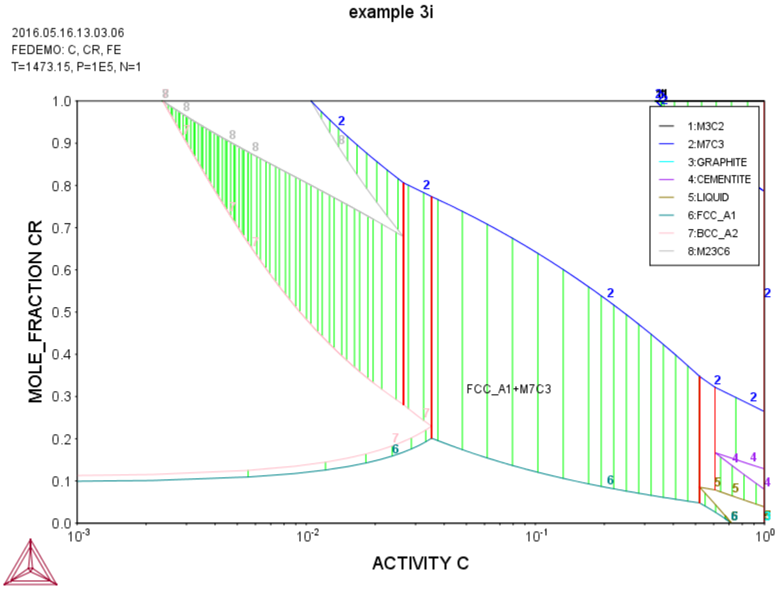
```
     For instance, the SIGMA, FCC, BCC and LIQUID phases (among others) in
     a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database)
     may be modeled by certain models, and their NA values must be evaluated
     in different ways, as described below:
       LIQUID      (C,Cr,CrO3/2,Fe,FeO,FEO3/2,N,Ni,NiO)1   --> NA = 1
       FCC_A1      (Cr,Fe,Ni)1(Va,C,N,O)1                  --> NA = 1
       BCC_A2      (Cr,Fe,Ni)1(Va,C,N,O)3                  --> NA = 1
       SIGMA       (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18               --> NA = 30
     If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase has been
     modeled by the Two-Sublattice Ionic Liquid Model, i.e.,
       IONIC_LIQ  (Cr+3,Fe+2,Ni+2)p(VA,C,N,O-2,FEO3/2)q
     the evaluation of its NA value becomes even more complicated,
       NA = p+q*y(C_2ndSite)+q*(N_2ndSite)+q*(O-2_2ndSite)+q*(FeO3/2_2ndSite)
     where the stoichiometric coefficients p and q are also dependent upon the
     real equilibrium state (rather than having fixed values in the system).
     Similar situations occur for other (solid) phases which are described by
     multiple-sublattice model with ionic constituents, such as SPINEL and
     HALITE phases in some databases.

   * Obviously, there will be no strange thing when using a zero value
     [i.e., 0] in a FIXED phase-status, since it simply means the specified
     phase is stable in equilibrium state but has a zero-amount of mass in
     the equilibrium calculations; in other words, on a phase diagram, the
     specific phase is on a zero-fraction line (ZFL), i.e., it just starts
     becoming stable on one side of a corresponding phase-boundary line or
     unstable on the other side of the same boundary. It is often and
     efficient to do so when calculating e.g. solidus equilibrium states.

   * However, when a non-zero value [it must always be positive; e.g., 1 or
     0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is
     unnecessarily the exactly same stable amount of the specific FIXED-
     status phase in a calculated equilibrium state any longer; instead,
     the <equilibrium amount> value is the "NPF(phase)" value that is only
     roughly used as the estimated starting-value of the FIXED-status phase
     in the equilibrium calculations.

     Therefore, a FIXED-status for a liquid phase being unity does not
     necessarily imply that it is a liquidus equilibrium state (where the
     liquid phase is in equilibrium with some solid phases but the liquid
     phase takes all the mass in the defined system). A unity value for
     setting the liquid phase status in calculating liquidus equilibrium
     state can only be used when the liquid mixture phase has been predefined
     as a single-sublattice solution phase (such as metallic liquid phase
     in multicomponent alloy systems) and the total system size as one mole
     (i.e., N=1).

     When a phase is described by a solution model in which two or more
     sublattices are considered and these sublattice sites may also have
     different stoichiometric coefficients [meaning that the mixture phase
     could have more than one atom in formula [NA>1; see some examples above],
     the unity value should not be used when setting the FIXED status for
     the phase; instead, one should use an appropriate value that ranges
     from 0 to a "NPF(phase)" value that equals to or is smaller than 1/NA
     (if the total system size N=1) or 1/NA*N (if N differs from unity).
     For this reason, if a multicomponent system bears an IONIC_LIQUID phase
     that is described by the Two-Sublattice Ionic Liquid Model (or any
     other multiple-sublattice ionic solution phases), it is very difficult
     to use a proper "NPF(ION_LIQ)" value in setting its FIXED phase-status,
     because that should be less than (or equal to) the complex value of
     N/[p+q*y(C_2ndSite)+q*(N_2ndSite)+q*(O-2_2ndSite)+q*(FeO3/2_2ndSite)].

Status: /ENTERED/: special
POLY_3:
POLY_3: post
POST:
POST: set-title example 3g
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Finally scale
POST: s-s x n .001 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 3h
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ This kind of diagram is useful to understand diffusion paths.
POST: @@
POST: @@ The phase labels were lost when we changed axis
POST: @@ One may add them again
POST: add .05 .3
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
Calculated         16532 grid points in             0 s
 Stable phases are: FCC_A1+M7C3
Text size: /.36/:
POST: set-title example 3i
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

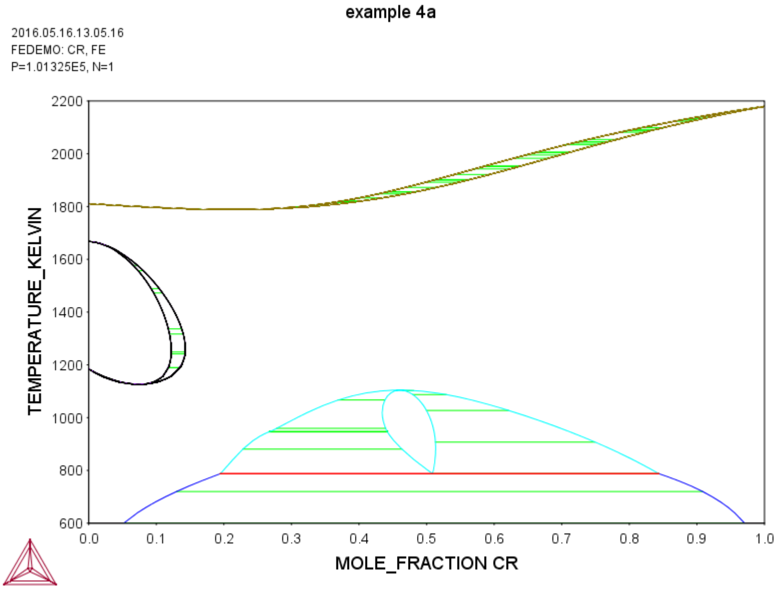
tcex04

```
About License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex04\tcex04.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of the miscibility gap in Fe-Cr
SYS: @@
SYS: set-log ex04,,,
SYS:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw FEDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys
   ... the command in full is DEFINE_SYSTEM
ELEMENTS: fe cr
 FE                       CR  DEFINED
TDB_FEDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 LIQUID:L    :CR FE:
 BCC_A2      :CR FE:VA:
 CHI_A12     :CR FE:CR:CR FE:
 FCC_A1      :CR FE:VA:
 HCP_A3      :CR FE:VA:
 LAVES_PHASE_C14 :CR FE:CR FE:
 SIGMA       :CR FE:CR:CR FE:
TDB_FEDEMO: rej ph /all
   ... the command in full is REJECT
 LIQUID:L                 BCC_A2                   CHI_A12
 FCC_A1                   HCP_A3                   LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 sigma
   ... the command in full is RESTORE
 LIQUID:L                 FCC_A1                   BCC_A2
 SIGMA  RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
TDB_FEDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 CR                       ENTERED   SER
 FE                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 SIGMA                    ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                   ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                   ENTERED      0.000000E+00    0.000000E+00
 LIQUID                   ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CR ENTERED    FE ENTERED    VA ENTERED
POLY_3:Hit RETURN to continue
POLY_3: @@ There is a miscibility gap in BCC Fe-Cr.
POLY_3: @@ Let us first calculate the low temperature region.
POLY_3: s-c x(cr)=.6 t=700 p=101325 n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          2230 grid points in              0 s
Found the set of lowest grid points in               0 s
 Creating a new composition set BCC_A2#2
 Calculated POLY solution       0 s, total time      0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: FEDEMO

 Conditions:
```

```
 X(CR)=0.6, T=700, P=1.01325E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    700.00 K (   426.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.35364E+01
 Total Gibbs energy -2.30658E+04,  Enthalpy  1.31794E+04,  Volume  7.26641E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      6.0000E-01  5.8274E-01 2.3703E-02 -2.1780E+04 SER
 FE                      4.0000E-01  4.1726E-01 1.3643E-02 -2.4995E+04 SER

 BCC_A2#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 6.0112E-01, Mass 3.1435E+01, Volume fraction 6.0312E-01  Mass fractions:
 CR  9.17570E-01  FE  8.24301E-02

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 3.9888E-01, Mass 2.2102E+01, Volume fraction 3.9688E-01  Mass fractions:
 FE  8.93484E-01  CR  1.06516E-01
POLY_3:Hit RETURN to continue
POLY_3: @@ Now make a calculation at a higher temperature
POLY_3: s-c t=900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          2230 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: FEDEMO

 Conditions:
 X(CR)=0.6, T=900, P=1.01325E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    900.00 K (   626.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.35364E+01
 Total Gibbs energy -3.49346E+04,  Enthalpy  2.36848E+04,  Volume  7.26400E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      6.0000E-01  5.8274E-01 1.2779E-02 -3.2626E+04 SER
 FE                      4.0000E-01  4.1726E-01 5.9088E-03 -3.8398E+04 SER

 SIGMA                       Status ENTERED     Driving force  0.0000E+00
 Moles 6.4245E-01, Mass 3.4609E+01, Volume fraction 6.3947E-01  Mass fractions:
 FE  5.04665E-01  CR  4.95335E-01

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 3.5755E-01, Mass 1.8927E+01, Volume fraction 3.6053E-01  Mass fractions:
 CR  7.42558E-01  FE  2.57442E-01
POLY_3:Hit RETURN to continue
POLY_3: @@ The Fe-Cr phase diagram has three non-connected two-phase regions.
POLY_3:
POLY_3: s-a-v 1 x(cr)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/:
POLY_3: s-a-v 2
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: t
Min value /0/: 600
Max value /1/: 2200
Increment /40/:
POLY_3: @@ Always a SAVE command before MAP (or STEP) unless
POLY_3: @@ you want to overlay this calculation with an earlier one
POLY_3: save tcex04 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Working hard

 Phase region boundary   1 at:   1.067E-02  1.169E+03
```

```
    BCC_A2
 ** FCC_A1
Calculated                     12  equilibria

Phase region boundary   2 at:   1.067E-02  1.169E+03
    BCC_A2
 ** FCC_A1
Calculated                     42  equilibria

Phase region boundary   3 at:   5.119E-01  6.100E+02
 ** BCC_A2
    BCC_A2#2
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary   4 at:   5.112E-01  6.000E+02
    BCC_A2
 ** BCC_A2#2
Calculated.                     10  equilibria

Phase region boundary   5 at:   5.192E-01  7.875E+02
    BCC_A2
 ** BCC_A2#2
 ** SIGMA

Phase region boundary   6 at:   6.763E-01  7.875E+02
    BCC_A2
 ** SIGMA
Calculated                     50  equilibria

Phase region boundary   7 at:   6.763E-01  7.875E+02
    BCC_A2
 ** SIGMA
Calculated.                    106  equilibria
Terminating at known equilibrium

Phase region boundary   8 at:   5.119E-01  6.100E+02
 ** BCC_A2
    BCC_A2#2
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary   9 at:   5.119E-01  6.100E+02
 ** BCC_A2
    BCC_A2#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  10 at:   5.119E-01  6.100E+02
 ** BCC_A2
    BCC_A2#2
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  11 at:   4.325E-02  1.137E+03
    BCC_A2
 ** FCC_A1
Calculated                     46  equilibria

Phase region boundary  12 at:   4.325E-02  1.137E+03
    BCC_A2
 ** FCC_A1
Calculated                     16  equilibria

Phase region boundary  13 at:   1.006E-01  1.137E+03
    BCC_A2
 ** FCC_A1
Calculated                     24  equilibria

Phase region boundary  14 at:   1.006E-01  1.137E+03
    BCC_A2
 ** FCC_A1
Calculated                     34  equilibria

Phase region boundary  15 at:   1.224E-02  1.663E+03
 ** BCC_A2
    FCC_A1
Calculated                     44  equilibria

Phase region boundary  16 at:   1.224E-02  1.663E+03
 ** BCC_A2
    FCC_A1
Calculated                     12  equilibria

Phase region boundary  17 at:   9.640E-03  1.809E+03
    LIQUID
 ** BCC_A2
Calculated                     11  equilibria

Phase region boundary  18 at:   9.640E-03  1.809E+03
    LIQUID
 ** BCC_A2
Calculated                     93  equilibria

Phase region boundary  19 at:   3.471E-01  1.807E+03
    LIQUID
 ** BCC_A2
Calculated                     37  equilibria

Phase region boundary  20 at:   3.471E-01  1.807E+03
    LIQUID
 ** BCC_A2
Calculated                     62  equilibria

Phase region boundary  21 at:   6.881E-01  2.007E+03
    LIQUID
 ** BCC_A2
Calculated                     68  equilibria

Phase region boundary  22 at:   6.881E-01  2.007E+03
    LIQUID
 ** BCC_A2
Calculated                     37  equilibria

Phase region boundary  23 at:   9.910E-01  2.176E+03
```

```
     LIQUID
  ** BCC_A2
 Calculated                      90  equilibria

 Phase region boundary  24 at:   9.910E-01  2.176E+03
     LIQUID
  ** BCC_A2
 Calculated                      12  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex04\tcex
 04.POLY3
 CPU time for mapping                       2  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST: s-t-s 6
   ... the command in full is SET_TIELINE_STATUS
POST: set_title example 4a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex05

```
SYS:About
 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex05\tcex05.TCM"SYS: set-echo
SYS:
SYS: @@ Calculation of a vertical section
SYS: @@ in the Al-Cu-Si system
SYS: @@ Calculation of a vertical section from Al to 10% cu2Si
SYS: @@
SYS: set-log ex05,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw ALDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Aluminum Demo Database

 VA                      /-  DEFINED
TDB_ALDEMO: def-sys al Cu si
   ... the command in full is DEFINE_SYSTEM
 AL                      CU                      SI
   DEFINED
TDB_ALDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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  'I. Ansara (Editor), COST 507, (1998)'
  'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),CU-Si'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'
  'C.-Y. He,Calphad, 33,200-210 (2009),Al-Cu-Si'
  'Volume data, N. Dupin 2008'
  'L. Kjellqvist, Thermo-Calc Software AB, 2010; Unassessed parameter,
      linear combination of unary volume data'
  'Hai-Lin Chen, in TCAL2.0, Extrapolations, assumptions
       adjustment'
  'J.R.Zhao, Y.Du, in , 2010, Sn-Sr, Cu-Mg-Si'
  'L. Kjellqvist, Thermo-Calc Software AB, 2012; Molar volumes'
  'W.H. Sun,unpublished (2010),Cu-Si-Zn,Cu-Ni-Zn'
 -OK-
TDB_ALDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1000,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY_3: @@ We shall calculate along a line where the cu content is twice
POLY_3: @@ that of the Si content, this can be used as a condition.
POLY_3: @@ Note that the whole equation must be given before the equal sign.
POLY_3: @@ It is wrong to write s-c x(cu)=2*x(si).
POLY_3: s-c x(cu)-2*x(si)=0
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1000, P=1E5, N=1, X(CU)-2*X(SI)=0
 DEGREES OF FREEDOM 1
POLY_3: s-c w(si)=0.05
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         16528 grid points in             0 s
   115 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: ALDEMO

 Conditions:
 T=1000, P=1E5, N=1, X(CU)-2*X(SI)=0, W(SI)=5E-2
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  3.10908E+01
 Total Gibbs energy -5.01533E+04,  Enthalpy  2.90243E+04,  Volume  1.00919E-05

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      8.3395E-01  7.2374E-01 4.7926E-03 -4.4405E+04 SER
 CU                      1.1070E-01  2.2626E-01 9.6970E-06 -9.5980E+04 SER
```
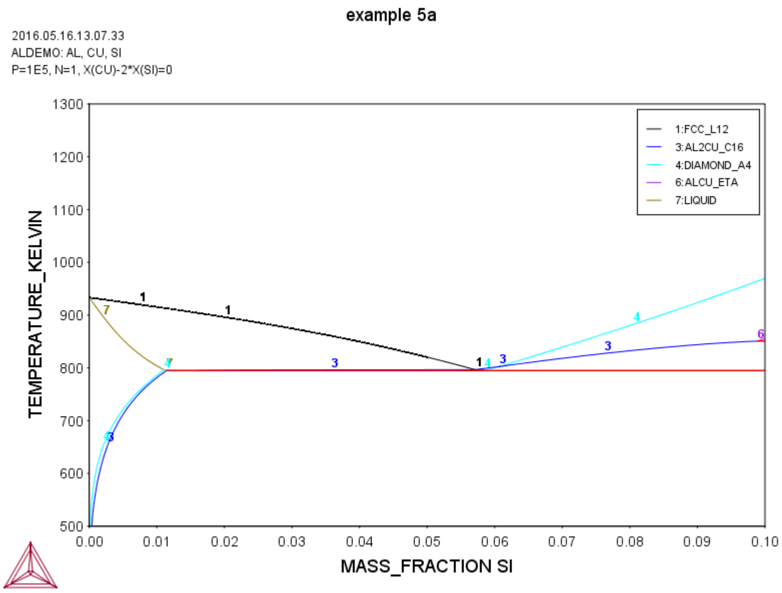
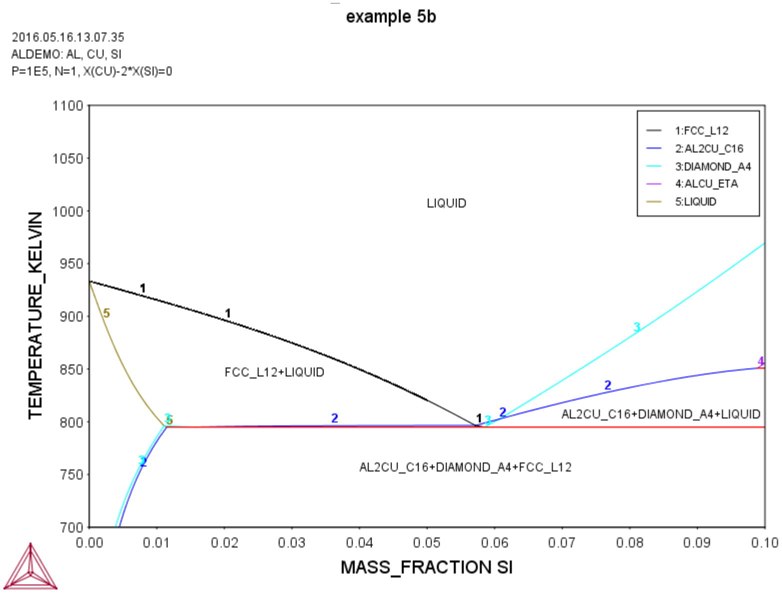

```
 SI                        5.5351E-02  5.0000E-02 4.4065E-03 -4.5103E+04 SER

 LIQUID                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.1091E+01, Volume fraction 1.0000E+00  Mass fractions:
 AL  7.23737E-01  CU  2.26263E-01  SI  5.00000E-02
POLY_3:@?<Hit_return_to_continue>
POLY_3: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  EXIT                      REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE               SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                      SELECT_EQUILIBRIUM
 BACK                     INFORMATION               SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE        SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS           SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM          SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA   SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS               SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS              SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM  SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN           SET_START_VALUE
 DELETE_SYMBOL            MAP                       SHOW_VALUE
 ENTER_SYMBOL             POST                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES           TABULATE
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(si)
Min value /0/: 0
Max value /1/: .1
Increment /.0025/: .0025
POLY_3: s-a-v 2
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: t
Min value /0/: 500
Max value /1/: 1300
Increment /20/: 10
POLY_3: l-a-v
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(SI)                  Min: 0         Max: 0.1       Inc: 2.5E-3
  Axis No 2: T                      Min: 500       Max: 1300      Inc: 10
POLY_3:@?<Hit_return_to_continue>
POLY_3: save tcex05 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16

 Phase region boundary   1 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated                      37  equilibria

 Phase region boundary   2 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated.                       4  equilibria

 Phase region boundary   3 at:   5.713E-02  7.965E+02
  ** AL2CU_C16
  ** FCC_L12
     LIQUID

 Phase region boundary   4 at:   5.713E-02  7.965E+02
     AL2CU_C16
  ** FCC_L12
     LIQUID
 Calculated.                       2  equilibria

 Phase region boundary   5 at:   5.852E-02  7.950E+02
     AL2CU_C16
  ** DIAMOND_A4
  ** FCC_L12
     LIQUID

 Phase region boundary   6 at:   1.036E-01  7.950E+02
     AL2CU_C16
     DIAMOND_A4
  ** FCC_L12

 Phase region boundary   7 at:   1.147E-02  7.950E+02
  ** AL2CU_C16
```

```
    DIAMOND_A4
    FCC_L12
Calculated..                     31  equilibria
Terminating at axis limit.

Phase region boundary   8 at:   1.036E-01  7.950E+02
    AL2CU_C16
    DIAMOND_A4
 ** LIQUID

Phase region boundary   9 at:   5.852E-02  7.950E+02
    AL2CU_C16
 ** DIAMOND_A4
    LIQUID
Calculated.                      2  equilibria

Phase region boundary  10 at:   6.069E-02  8.026E+02
 ** AL2CU_C16
 ** DIAMOND_A4
    LIQUID

Phase region boundary  11 at:   6.069E-02  8.026E+02
 ** DIAMOND_A4
    LIQUID
Calculated..                     18  equilibria
Terminating at axis limit.

Phase region boundary  12 at:   6.069E-02  8.026E+02
 ** AL2CU_C16
    LIQUID
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  13 at:   6.069E-02  8.026E+02
 ** AL2CU_C16
    DIAMOND_A4
    LIQUID
Calculated.                     22  equilibria

Phase region boundary  14 at:   9.890E-02  8.509E+02
 ** AL2CU_C16
 ** ALCU_ETA
    DIAMOND_A4
    LIQUID

Phase region boundary  15 at:   1.058E-01  8.509E+02
    AL2CU_C16
 ** ALCU_ETA
    DIAMOND_A4

Phase region boundary  16 at:   1.350E-01  8.509E+02
 ** AL2CU_C16
    ALCU_ETA
    DIAMOND_A4

Phase region boundary  17 at:   1.058E-01  8.509E+02
    AL2CU_C16
    DIAMOND_A4
 ** LIQUID

Phase region boundary  18 at:   1.350E-01  8.509E+02
    ALCU_ETA
    DIAMOND_A4
 ** LIQUID

Phase region boundary  19 at:   9.890E-02  8.509E+02
 ** ALCU_ETA
    DIAMOND_A4
    LIQUID
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary  20 at:   1.581E-02  7.950E+02
 ** AL2CU_C16
    FCC_L12
    LIQUID
Calculated.                     18  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   1.147E-02  7.950E+02
    DIAMOND_A4
    FCC_L12
 ** LIQUID
Calculated.                      2  equilibria

Phase region boundary  22 at:   1.107E-02  7.962E+02
 ** DIAMOND_A4
    FCC_L12
 ** LIQUID

Phase region boundary  23 at:   1.107E-02  7.962E+02
    FCC_L12
 ** LIQUID
Calculated                     24  equilibria

Phase region boundary  24 at:   1.107E-02  7.962E+02
 ** DIAMOND_A4
    FCC_L12
Calculated..                     31  equilibria
Terminating at axis limit.

Phase region boundary  25 at:   1.107E-02  7.962E+02
 ** DIAMOND_A4
    FCC_L12
    LIQUID
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   5.713E-02  7.965E+02
 ** FCC_L12
    LIQUID
Calculated                     43  equilibria

Phase region boundary  27 at:   5.000E-02  8.204E+02
 ** FCC_L12
    LIQUID
```

```
 Calculated                      37  equilibria

 Phase region boundary  28 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  29 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated                      37  equilibria

 Phase region boundary  30 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated                      37  equilibria

 Phase region boundary  32 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  33 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated                      37  equilibria

 Phase region boundary  34 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  35 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated                      37  equilibria

 Phase region boundary  36 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated                      37  equilibria

 Phase region boundary  38 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated                      37  equilibria

 Phase region boundary  40 at:   5.000E-02  8.204E+02
  ** FCC_L12
     LIQUID
 Calculated.                       4  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex05\tcex
 05.POLY3
 CPU time for mapping                      9  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: b
POST:
POST:
POST: set-title example 5a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:@?<Hit_return_to_continue>
POST: s-s y n 700 1100
   ... the command in full is SET_SCALING_STATUS
POST: @@ Note that the three-phase region LIQ-Si-Al2Cu is an area and not
POST: @@ a single line as in a binary system.  This is called a pseudo-binary section
POST: add .05 1000
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Stable phases are: LIQUID
Text size: /.36/:
POST: add .02 840
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
Calculated         16528 grid points in             0 s
 Stable phases are: FCC_L12+LIQUID
Text size: /.36/:
POST: add .04 750
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
Calculated         16528 grid points in             0 s
 Stable phases are: AL2CU_C16+DIAMOND_A4+FCC_L12
Text size: /.36/:
POST: add .07 800
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
Calculated         16528 grid points in             0 s
 Stable phases are: AL2CU_C16+DIAMOND_A4+LIQUID
Text size: /.36/:
POST:
POST: set-title example 5b
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:@?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex06

```
SYS:AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex06\tcex06.TCM"SYS: set-echo
SYS: @@
SYS: @@ Calculation of an isopleth in low alloyed
SYS: @@ Fe-Mn-Si-Cr-Ni-C steel. Calculation of a
SYS: @@ multicomponent phase diagram.
SYS: @@
SYS: set-log ex06,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ we use the define-material command in POLY and the TCFE steel database
POLY_3: @@ The material contains  1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C
POLY_3: @@ (by weight). These conditions are set by the command and in
POLY_3: @@ addition the temperature. Hidden commands set the pressure to 1 bar
POLY_3: @@ and that iron is "the rest".
POLY_3: @@ After calculating the first equilibrium we calculate a phase diagram
POLY_3: @@ with one axis variable as temperature and the other as the
POLY_3: @@ carbon content
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: ?

 Major element or alloy

  The material must have a "major" element, usually the element which is
  present in the largest amount. The fraction of this element will not be
  set but be "the rest".

  In some databases there are the "alloys" predefined. An alloy has a
  default major element and have limits of the amounts of the alloying
  elements. If the user stays within there limits the calculation should
  give reasonable results.


Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: y
1st alloying element: c
Mass (weight) percent /1/: 1
2nd alloying element: si .3
Next alloying element: mn .4
Next alloying element: ni 3.5
Next alloying element: cr 1.5
Next alloying element:
Temperature (C) /1000/: 1000
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M5C2                     M3C2
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 FE4N_LP1                 FECN_CHI                 SIGMA
 CHI_A12                  LAVES_PHASE_C14          M3SI
 G_PHASE                  CR3SI                    FE2SI
 MSI                      M5SI3                    NBNI3
 NI3TI                    AL4C3                    FE8SI2C
 SIC

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

 ........................................................

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M5C2                     M3C2
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 FE4N_LP1                 FECN_CHI                 SIGMA
 CHI_A12                  LAVES_PHASE_C14          M3SI
 G_PHASE                  CR3SI                    FE2SI
 MSI                      M5SI3                    NBNI3
 NI3TI                    AL4C3                    FE8SI2C
 SIC

 ........................................................

OK? /Y/: Y
```

```
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

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 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         23376 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY_3:
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
```
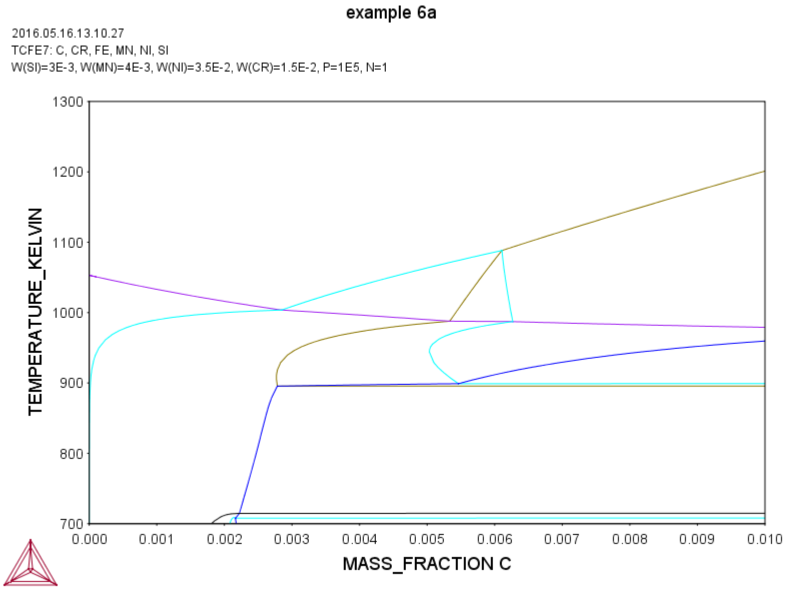

```
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1273.15, W(C)=1E-2, W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2,
    P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1273.15 K (  1000.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.37536E+01
 Total Gibbs energy -6.46529E+04,  Enthalpy  3.76283E+04,  Volume  7.13756E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.4754E-02  1.0000E-02 8.3878E-02 -2.6235E+04 SER
 CR                      1.5507E-02  1.5000E-02 1.2598E-04 -9.5052E+04 SER
 FE                      8.9803E-01  9.3300E-01 2.4771E-03 -6.3521E+04 SER
 MN                      3.9138E-03  4.0000E-03 3.0765E-06 -1.3435E+05 SER
 NI                      3.2056E-02  3.5000E-02 6.1631E-05 -1.0262E+05 SER
 SI                      5.7417E-03  3.0000E-03 6.4662E-09 -1.9961E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3754E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  9.33000E-01  CR  1.50000E-02  MN  4.00000E-03
 NI  3.50000E-02  C   1.00000E-02  SI  3.00000E-03
POLY_3:Hit RETURN to continue
POLY_3: @@ Note that values now must be set in fractions and Kelvin!
POLY_3: @@ Sorry about that
POLY_3: s-a-v 1 w(c)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .01
Increment /2.5E-04/: 1E-4
POLY_3: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 700
Max value /1/: 1300
Increment /15/:
POLY_3: save tcex06 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   1.953E-03  7.100E+02
     BCC_A2
     FCC_A1
  ** M3C2
     M7C3
 Calculated..                        3  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   1.810E-03  7.000E+02
     BCC_A2
     FCC_A1
  ** M3C2
     M7C3
 Calculated.                       10  equilibria

 Phase region boundary   3 at:   2.222E-03  7.146E+02
     BCC_A2
     FCC_A1
  ** GRAPHITE
  ** M3C2
     M7C3

 Phase region boundary   4 at:   2.222E-03  7.146E+02
     BCC_A2
     FCC_A1
     GRAPHITE
```

```
 ** M3C2
    M7C3
Calculated..                     80  equilibria
Terminating at axis limit.

Phase region boundary   5 at:   2.222E-03  7.146E+02
    BCC_A2
    FCC_A1
 ** GRAPHITE
    M7C3
Calculated.                     21  equilibria

Phase region boundary   6 at:   2.784E-03  8.955E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
 ** GRAPHITE
    M7C3

Phase region boundary   7 at:   2.784E-03  8.955E+02
    BCC_A2
    CEMENTITE
    FCC_A1
 ** GRAPHITE
    M7C3
Calculated.                     28  equilibria

Phase region boundary   8 at:   5.463E-03  8.990E+02
    BCC_A2
    CEMENTITE
    FCC_A1
 ** GRAPHITE
 ** M7C3

Phase region boundary   9 at:   5.463E-03  8.990E+02
    BCC_A2
    CEMENTITE
    FCC_A1
 ** GRAPHITE
Calculated..                     48  equilibria
Terminating at axis limit.

Phase region boundary  10 at:   5.463E-03  8.990E+02
    BCC_A2
    CEMENTITE
    FCC_A1
 ** M7C3
Calculated.                     22  equilibria

Phase region boundary  11 at:   6.268E-03  9.872E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1
 ** M7C3

Phase region boundary  12 at:   6.268E-03  9.872E+02
    CEMENTITE
    FCC_A1
 ** M7C3
Calculated.                      8  equilibria

Phase region boundary  13 at:   6.107E-03  1.088E+03
 ** CEMENTITE
    FCC_A1
 ** M7C3

Phase region boundary  14 at:   6.107E-03  1.088E+03
    FCC_A1
 ** M7C3
Calculated.                     34  equilibria

Phase region boundary  15 at:   2.846E-03  1.004E+03
 ** BCC_A2
    FCC_A1
 ** M7C3

Phase region boundary  16 at:   2.846E-03  1.004E+03
    BCC_A2
    FCC_A1
 ** M7C3
Calculated..                     53  equilibria
Terminating at axis limit.

Phase region boundary  17 at:   2.846E-03  1.004E+03
 ** BCC_A2
    FCC_A1
Calculated                     41  equilibria

Phase region boundary  18 at:   2.846E-03  1.004E+03
 ** BCC_A2
    FCC_A1
    M7C3
Calculated.                     26  equilibria

Phase region boundary  19 at:   5.334E-03  9.878E+02
 ** BCC_A2
 ** CEMENTITE
    FCC_A1
    M7C3

Phase region boundary  20 at:   5.334E-03  9.878E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1
    M7C3
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   5.334E-03  9.878E+02
 ** CEMENTITE
    FCC_A1
    M7C3
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   5.334E-03  9.878E+02
```

```
    BCC_A2
 ** CEMENTITE
    FCC_A1
    M7C3
Calculated.                     36  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   6.107E-03  1.088E+03
 ** CEMENTITE
    FCC_A1
Calculated..                     41  equilibria
Terminating at axis limit.

Phase region boundary  24 at:   6.268E-03  9.872E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1
Calculated..                     40  equilibria
Terminating at axis limit.

Phase region boundary  25 at:   5.463E-03  8.990E+02
    BCC_A2
    CEMENTITE
    FCC_A1
    GRAPHITE
 ** M7C3
Calculated..                     48  equilibria
Terminating at axis limit.

Phase region boundary  26 at:   2.784E-03  8.955E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
    GRAPHITE
    M7C3
Calculated..                     75  equilibria
Terminating at axis limit.

Phase region boundary  27 at:   2.222E-03  7.146E+02
    BCC_A2
    FCC_A1
 ** GRAPHITE
    M3C2
    M7C3
Calculated.                      2  equilibria

Phase region boundary  28 at:   2.164E-03  7.078E+02
    BCC_A2
    FCC_A1
 ** GRAPHITE
    M3C2
 ** M7C3

Phase region boundary  29 at:   2.164E-03  7.078E+02
    BCC_A2
    FCC_A1
 ** GRAPHITE
    M3C2
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary  30 at:   2.164E-03  7.078E+02
    BCC_A2
    FCC_A1
    M3C2
 ** M7C3
Calculated..                     16  equilibria
Terminating at axis limit.

Phase region boundary  31 at:   2.164E-03  7.078E+02
    BCC_A2
    FCC_A1
    GRAPHITE
    M3C2
 ** M7C3
Calculated..                     81  equilibria
Terminating at axis limit.

Phase region boundary  32 at:   1.953E-03  7.100E+02
    BCC_A2
    FCC_A1
 ** M3C2
    M7C3
Calculated.                      7  equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   1.000E-04  9.417E+02
    BCC_A2
    FCC_A1
 ** M7C3
Calculated..                     26  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  34 at:   1.000E-04  9.417E+02
    BCC_A2
    FCC_A1
 ** M7C3
Calculated.                     29  equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   3.367E-03  7.146E+02
    BCC_A2
    FCC_A1
    GRAPHITE
 ** M3C2
    M7C3
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  36 at:   3.367E-03  7.146E+02
    BCC_A2
    FCC_A1
    GRAPHITE
 ** M3C2
    M7C3
```

```
Calculated..                     69  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  37 at:   6.633E-03  7.147E+02
    BCC_A2
    FCC_A1
    GRAPHITE
 ** M3C2
    M7C3
Calculated.                     46  equilibria
Terminating at known equilibrium

Phase region boundary  38 at:   6.633E-03  7.147E+02
    BCC_A2
    FCC_A1
    GRAPHITE
 ** M3C2
    M7C3
Calculated..                     36  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  39 at:   2.185E-03  7.100E+02
    BCC_A2
    FCC_A1
 ** GRAPHITE
    M3C2
    M7C3
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   2.185E-03  7.100E+02
    BCC_A2
    FCC_A1
 ** GRAPHITE
    M3C2
    M7C3
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   9.900E-03  7.148E+02
    BCC_A2
    FCC_A1
    GRAPHITE
 ** M3C2
    M7C3
Calculated.                     78  equilibria
Terminating at known equilibrium

Phase region boundary  42 at:   9.900E-03  7.148E+02
    BCC_A2
    FCC_A1
    GRAPHITE
 ** M3C2
    M7C3
Calculated..                      3  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  43 at:   2.772E-03  9.033E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
    M7C3
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  44 at:   2.772E-03  9.033E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
    M7C3
Calculated.                     32  equilibria
Terminating at known equilibrium

Phase region boundary  45 at:   5.632E-03  9.033E+02
    BCC_A2
    CEMENTITE
    FCC_A1
 ** GRAPHITE
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  46 at:   5.632E-03  9.033E+02
    BCC_A2
    CEMENTITE
    FCC_A1
 ** GRAPHITE
Calculated..                     46  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  47 at:   6.376E-03  1.097E+03
 ** CEMENTITE
    FCC_A1
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  48 at:   6.376E-03  1.097E+03
 ** CEMENTITE
    FCC_A1
Calculated..                     39  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  49 at:   6.376E-03  1.097E+03
 ** CEMENTITE
    FCC_A1
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  50 at:   6.376E-03  1.097E+03
 ** CEMENTITE
    FCC_A1
Calculated..                     39  equilibria
```

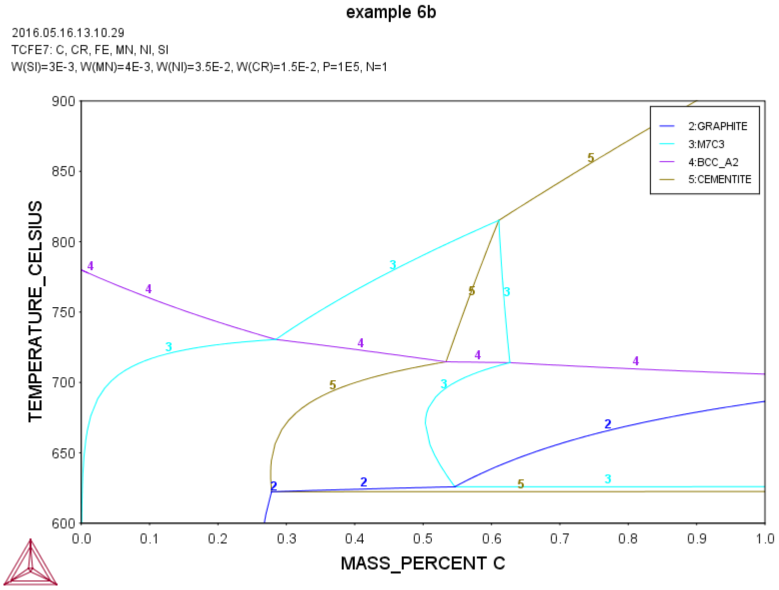
```
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  51 at:   1.000E-04  1.051E+03
  ** BCC_A2
     FCC_A1
 Calculated                        4  equilibria

 Phase region boundary  52 at:   1.000E-04  1.051E+03
  ** BCC_A2
     FCC_A1
 Calculated.                      29  equilibria
 Terminating at known equilibrium

 Phase region boundary  53 at:   3.367E-03  1.020E+03
     FCC_A1
  ** M7C3
 Calculated.                       7  equilibria
 Terminating at known equilibrium

 Phase region boundary  54 at:   3.367E-03  1.020E+03
     FCC_A1
  ** M7C3
 Calculated.                      29  equilibria
 Terminating at known equilibrium

 Phase region boundary  55 at:   6.633E-03  1.105E+03
  ** CEMENTITE
     FCC_A1
 Calculated.                       7  equilibria
 Terminating at known equilibrium

 Phase region boundary  56 at:   6.633E-03  1.105E+03
  ** CEMENTITE
     FCC_A1
 Calculated..                      36  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  57 at:   9.900E-03  1.198E+03
  ** CEMENTITE
     FCC_A1
 Calculated.                      39  equilibria
 Terminating at known equilibrium

 Phase region boundary  58 at:   9.900E-03  1.198E+03
  ** CEMENTITE
     FCC_A1
 Calculated..                       4  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex06\tcex
 06.POLY3
 CPU time for mapping                      34  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: set-title example 6a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```


example 6a

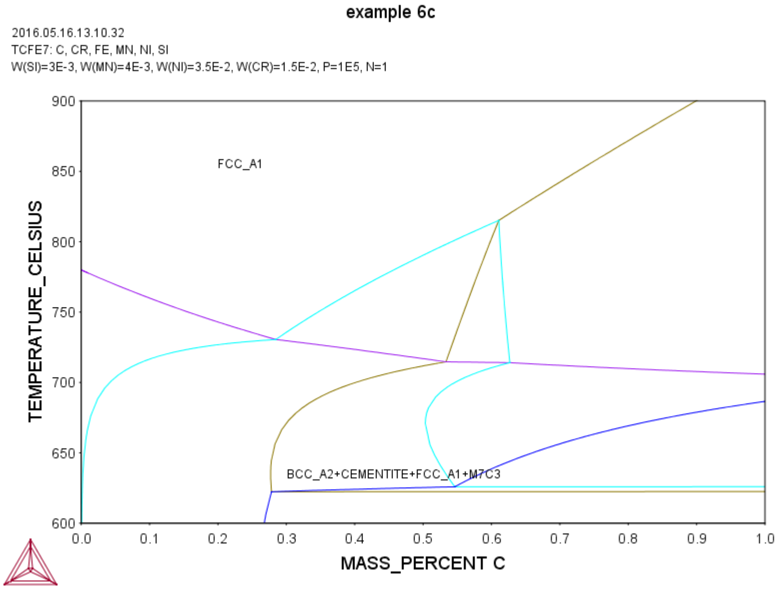
2016.05.16.13.10.27
TCFE7: C, CR, FE, MN, NI, SI
W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2, P=1E5, N=1

```
POST:
POST:Hit RETURN to continue
POST: @@ Use more practical quantities in the plot and
POST: @@ label the curves
POST: s-d-a x w-p c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST:
POST: s-s y n 600 900
   ... the command in full is SET_SCALING_STATUS
POST:
POST: s-lab b
```

```
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Determine the phase region at the iron rich side
POST: add .2 850
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated         23376 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: FCC_A1
Text size: /.36/:
POST: @@ Knowing that only FCC (or austenite) is stable in that region and
POST: @@ which phase is stable along each line, one can determine the phases
POST: @@ in each region. For example at 0.3 % C and 630 degree C one should
POST: @@ have FCC+BCC+M7C3+CEMENTITE.
POST: @@ Check by adding a label
POST: add .3 630
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated         23376 grid points in              1 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      1  s
 Stable phases are: BCC_A2+CEMENTITE+FCC_A1+M7C3
Text size: /.36/:
POST: s-lab n
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex07

```
About Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex07\tcex07.TCM"SYS: set-echo
SYS: @@
SYS: @@ Calculation
SYS: @@ of single equilibria in low alloyed
SYS: @@ Fe-Mn-Si-Cr-Ni-C steel.
SYS: @@
SYS: @@ Single equilibrium calculations in a steel.
SYS: @@
SYS: @@ There are two common ways to perform a single equilibrium calculation.
SYS: @@ 1) start from scratch: firstly get data from database, then in
SYS: @@    POLY use SET_CONDITION and COMPUTE_EQUILIBRIUM.
SYS: @@ 2) Go directly to POLY, and use DEFINE_MATERIAL.
SYS: @@
SYS: @@ One often wants to know the temperature or composition where one phase
SYS: @@ forms or disappears, COMPUTE_TRANSITION is a useful command. It is the
SYS: @@ same as the CHANGE_STATUS/SET_CONDITION/COMPUTE_EQUILIBRIUM combination.
SYS: @@
SYS: set-log ex07,,
SYS: @@ The alloy composition is 1 wt% Cr, 0.3 wt% Si, 0.3wt% Mn,
SYS: @@ 2.8 wt% Ni and 0.55 wt% C
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .55
2nd alloying element: cr 1
Next alloying element: mn .3 ni 2.8 si .3
Next alloying element:
Temperature (C) /1000/: 600
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M5C2                     M3C2
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 FE4N_LP1                 FECN_CHI                 SIGMA
 CHI_A12                  LAVES_PHASE_C14          M3SI
 G_PHASE                  CR3SI                    FE2SI
 MSI                      M5SI3                    NBNI3
 NI3TI                    AL4C3                    FE8SI2C
 SIC

Reject phase(s) /NONE/:
Restore phase(s): /NONE/:

 ........................................................

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M5C2                     M3C2
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 FE4N_LP1                 FECN_CHI                 SIGMA
 CHI_A12                  LAVES_PHASE_C14          M3SI
 G_PHASE                  CR3SI                    FE2SI
 MSI                      M5SI3                    NBNI3
 NI3TI                    AL4C3                    FE8SI2C
 SIC

 ........................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
```

```
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

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 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         23376 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: @@ The first equilibrium is calculated automatically
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
```
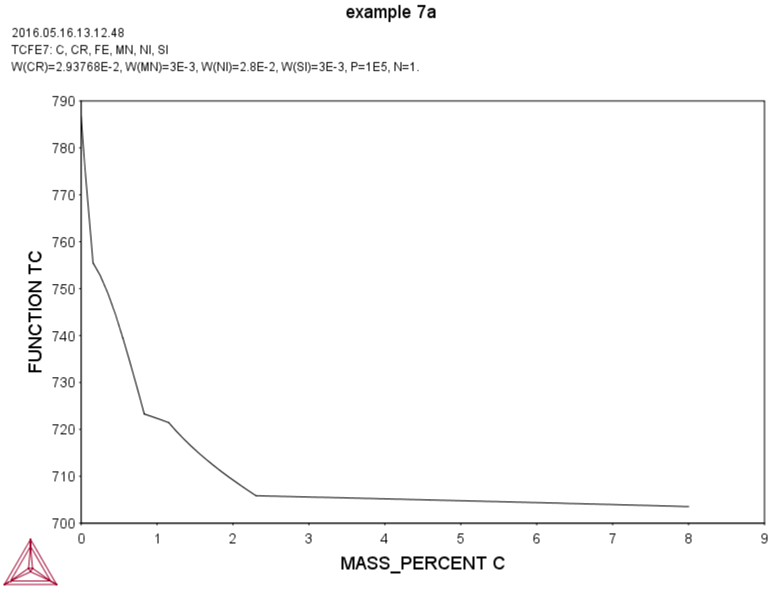

```
 T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,
    P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    873.15 K (   600.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.46196E+01
 Total Gibbs energy -3.56732E+04,  Enthalpy  1.79282E+04,  Volume  7.20787E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        2.5011E-02  5.5000E-03 2.6153E-01 -9.7369E+03 SER
 CR                       1.0505E-02  1.0000E-02 2.4479E-04 -6.0366E+04 SER
 FE                       9.2961E-01  9.5050E-01 8.6789E-03 -3.4461E+04 SER
 MN                       2.9826E-03  3.0000E-03 2.8925E-05 -7.5871E+04 SER
 NI                       2.6058E-02  2.8000E-02 3.4662E-04 -5.7841E+04 SER
 SI                       5.8342E-03  3.0000E-03 2.9885E-11 -1.7593E+05 SER

 BCC_A2                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.5814E-01, Mass 5.3405E+01, Volume fraction 9.6729E-01  Mass fractions:
 FE  9.63504E-01  SI  3.06820E-03  MN  2.28601E-03
 NI  2.85952E-02  CR  2.52703E-03  C   1.97123E-05

 M7C3                         Status ENTERED     Driving force  0.0000E+00
 Moles 2.4194E-02, Mass 1.0019E+00, Volume fraction 1.9532E-02  Mass fractions:
 FE  4.58650E-01  C   8.70086E-02  NI  2.20485E-03
 CR  4.10444E-01  MN  4.16928E-02  SI  3.04624E-12

 GRAPHITE                     Status ENTERED     Driving force  0.0000E+00
 Moles 1.7665E-02, Mass 2.1218E-01, Volume fraction 1.3181E-02  Mass fractions:
 C   1.00000E+00  NI  0.00000E+00  FE  0.00000E+00
 SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
POLY_3: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  EXIT                      REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE               SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                      SELECT_EQUILIBRIUM
 BACK                     INFORMATION               SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE        SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS           SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM          SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA   SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS               SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS              SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM  SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN           SET_START_VALUE
 DELETE_SYMBOL            MAP                       SHOW_VALUE
 ENTER_SYMBOL             POST                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES           TABULATE
POLY_3:Hit RETURN to continue
POLY_3: @@ Increase Cr until all Graphite disappears. Calculate this
POLY_3: @@ directly using the COMPUTE-TRANSITION command.  You
POLY_3: @@ must release the Cr content of course
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: grap
 You must release one of these conditions
 T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,
 P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: w(cr)
 Testing POLY result by global minimization procedure
 Using already calculated grid
To form GRAP the condition is set to W(CR)=.0293768365613
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=873.15, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
    W(SI)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    873.15 K (   600.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45430E+01
 Total Gibbs energy -3.61950E+04,  Enthalpy  1.77828E+04,  Volume  7.15532E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        2.4976E-02  5.5000E-03 2.6153E-01 -9.7369E+03 SER
 CR                       3.0816E-02  2.9377E-02 2.5353E-04 -6.0112E+04 SER
 FE                       9.0938E-01  9.3112E-01 8.6730E-03 -3.4466E+04 SER
 MN                       2.9784E-03  3.0000E-03 1.8254E-05 -7.9213E+04 SER
 NI                       2.6022E-02  2.8000E-02 3.6127E-04 -5.7540E+04 SER
 SI                       5.8260E-03  3.0000E-03 3.1190E-11 -1.7562E+05 SER

 BCC_A2                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.1702E-01, Mass 5.1110E+01, Volume fraction 9.3250E-01  Mass fractions:
 FE  9.62968E-01  SI  3.20151E-03  MN  1.45355E-03
 NI  2.97317E-02  CR  2.62575E-03  C   1.94050E-05

 M7C3                         Status ENTERED     Driving force  0.0000E+00
 Moles 8.2978E-02, Mass 3.4330E+00, Volume fraction 6.7498E-02  Mass fractions:
 FE  4.57021E-01  C   8.70942E-02  NI  2.21880E-03
 CR  4.27642E-01  MN  2.60233E-02  SI  3.17758E-12

 GRAPHITE                     Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 C   1.00000E+00  NI  0.00000E+00  FE  0.00000E+00
 SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Graphite disappears when we have this chromium content 2.94 w/o
POLY_3: @@ The amount of Cr can be obtain directly with a show command
POLY_3: show w(cr)
   ... the command in full is SHOW_VALUE
 W(CR)=2.9376837E-2
POLY_3: @@ This is automatically set as new condition by the C-T command
POLY_3: @@ and the amount of graphite is zero.
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 M7C3                     ENTERED      0.000000E+00    8.297805E-02
 GRAPHITE                 ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                   ENTERED      0.000000E+00    9.170220E-01
```

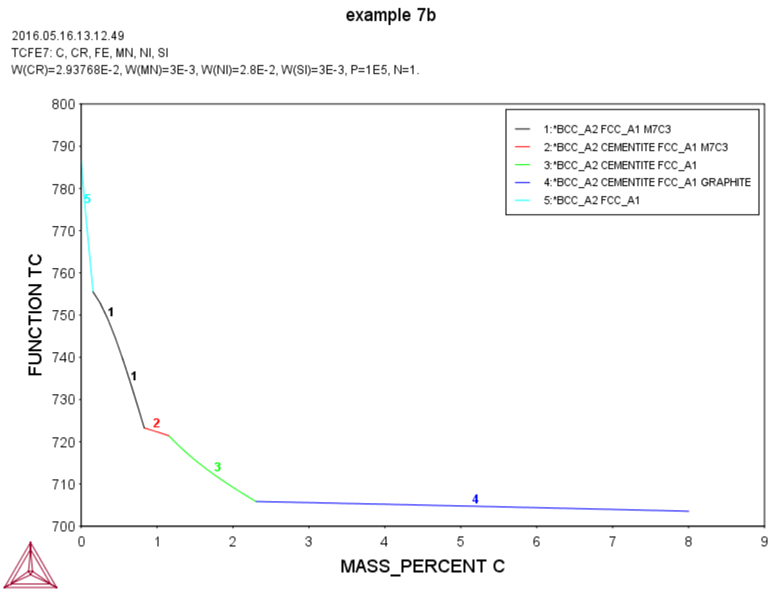
```
 CEMENTITE               ENTERED     -1.684846E-02    0.000000E+00
 FCC_A1                  ENTERED     -1.785775E-02    0.000000E+00
 FCC_A1#2                ENTERED     -1.785775E-02    0.000000E+00
 M23C6                   ENTERED     -9.187797E-02    0.000000E+00
 KAPPA                   ENTERED     -1.728791E-01    0.000000E+00
 M3C2                    ENTERED     -2.522305E-01    0.000000E+00
 HCP_A3                  ENTERED     -2.617842E-01    0.000000E+00
 HCP_A3#2                ENTERED     -2.617842E-01    0.000000E+00
 FECN_CHI                ENTERED     -3.867251E-01    0.000000E+00
 M5C2                    ENTERED     -5.597293E-01    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -6.753681E-01
 LIQUID SIGMA CHI_A12 DIAMOND_FCC_A4 FE4N_LP1 LAVES_PHASE_C14 KSI_CARBIDE
 FE8SI2C G_PHASE M3SI NI3TI FE2SI NBNI3 CR3SI M5SI3 MSI SIC AL4C3 GAS
POLY_3: @@ Now determine the maximum temperature with no Austenite (FCC_A1),
POLY_3: @@ i.e. A1 temperature.
POLY_3: @@ We use again the new command COMPUTE-TRANSITION
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: fcc_a1
 You must release one of these conditions
 T=873.15, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
 W(SI)=3E-3, P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
 Testing POLY result by global minimization procedure
Calculated         23376 grid points in             0 s
To form FCC_A1 the condition is set to T=915.22062277
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
    W(SI)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY_3: @@ This command does the same as the change-status/set-cond/compute-equil,
POLY_3: @@ Notice that the temperature is set back as condition with the new value.
POLY_3: @@ If we want temperatures in Celsius we can enter a function.
POLY_3: ent fun tc=t-273;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh tc
   ... the command in full is SHOW_VALUE
 TC=642.22062
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
    W(SI)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    915.22 K (   642.07 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45430E+01
 Total Gibbs energy -3.88407E+04,  Enthalpy  1.96981E+04,  Volume  7.16989E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.4976E-02  5.5000E-03 2.1560E-01 -1.1676E+04 SER
 CR                      3.0816E-02  2.9377E-02 2.6256E-04 -6.2742E+04 SER
 FE                      9.0938E-01  9.3112E-01 7.6560E-03 -3.7076E+04 SER
 MN                      2.9784E-03  3.0000E-03 1.5918E-05 -8.4071E+04 SER
 NI                      2.6022E-02  2.8000E-02 2.9594E-04 -6.1831E+04 SER
 SI                      5.8260E-03  3.0000E-03 6.4895E-11 -1.7851E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.1724E-01, Mass 5.1116E+01, Volume fraction 9.3276E-01  Mass fractions:
 FE  9.61872E-01  CR  3.48152E-03  MN  1.68770E-03
 NI  2.97230E-02  SI  3.20115E-03  C   3.45703E-05

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 8.2763E-02, Mass 3.4273E+00, Volume fraction 6.7240E-02  Mass fractions:
 FE  4.72522E-01  C   8.70137E-02  NI  2.30172E-03
 CR  4.15590E-01  MN  2.25722E-02  SI  8.20561E-12

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.68031E-01  MN  1.44441E-02  SI  4.18888E-03
 NI  1.05328E-01  CR  5.51928E-03  C   2.48820E-03
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: cps
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 NI                      ENTERED   SER
 SI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 M7C3                    ENTERED      0.000000E+00    8.276289E-02
 FCC_A1                  ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                  ENTERED      0.000000E+00    9.172371E-01
 FCC_A1#2                ENTERED     -5.216451E-09    0.000000E+00
 CEMENTITE               ENTERED     -6.422721E-03    0.000000E+00
 M23C6                   ENTERED     -7.334991E-02    0.000000E+00
 GRAPHITE                ENTERED     -1.327548E-01    0.000000E+00
 KAPPA                   ENTERED     -1.370531E-01    0.000000E+00
 HCP_A3                  ENTERED     -2.513814E-01    0.000000E+00
 HCP_A3#2                ENTERED     -2.513814E-01    0.000000E+00
 M3C2                    ENTERED     -3.041886E-01    0.000000E+00
 FECN_CHI                ENTERED     -3.826414E-01    0.000000E+00
 M5C2                    ENTERED     -5.420475E-01    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -5.841299E-01
 LIQUID SIGMA CHI_A12 LAVES_PHASE_C14 FE4N_LP1 DIAMOND_FCC_A4 KSI_CARBIDE
 FE8SI2C G_PHASE M3SI FE2SI NI3TI NBNI3 M5SI3 CR3SI MSI SIC AL4C3 GAS
 *** STATUS FOR ALL SPECIES
 C   ENTERED    C4  ENTERED    CR  ENTERED    NI  ENTERED
 C2  ENTERED    C5  ENTERED    FE  ENTERED    SI  ENTERED
 C3  ENTERED    C60 ENTERED    MN  ENTERED    VA  ENTERED
POLY_3: @@ Now determine maximum temperature where no Ferrite (BCC_A2) exists
```

```
POLY_3: @@ Use
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
You want to find when the current major phase is formed, please give
New major phase: fcc_a1
 You must release one of these conditions
 T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
 W(SI)=3E-3, P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
 Testing POLY result by global minimization procedure
Calculated         23376 grid points in             1 s
To form BCC_A2 the condition is set to T=1012.45181314
POLY_3:
POLY_3: show tc
   ... the command in full is SHOW_VALUE
 TC=739.45181
POLY_3:Hit RETURN to continue
POLY_3: @@ Check how this varies with the carbon content
POLY_3: ch-st phase fcc_a1
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: ent
Start value, number of moles /0/: 1
POLY_3: ch-st phase bcc_a2
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: fix
Number of moles /0/: 0
POLY_3:
POLY_3: s-c t=none
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         23376 grid points in             0 s
     7 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3, P=1E5,
    N=1
 FIXED PHASES
 BCC_A2=0
 DEGREES OF FREEDOM 0

 Temperature   1012.45 K (   739.30 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45430E+01
 Total Gibbs energy -4.54060E+04,  Enthalpy  2.77487E+04,  Volume  7.08402E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.4976E-02  5.5000E-03 7.8817E-02 -2.1387E+04 SER
 CR                      3.0816E-02  2.9377E-02 4.6417E-04 -6.4611E+04 SER
 FE                      9.0938E-01  9.3112E-01 5.7861E-03 -4.3372E+04 SER
 MN                      2.9784E-03  3.0000E-03 4.5168E-06 -1.0361E+05 SER
 NI                      2.6022E-02  2.8000E-02 8.0605E-05 -7.9348E+04 SER
 SI                      5.8260E-03  3.0000E-03 3.6734E-10 -1.8288E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.6176E-01, Mass 5.2968E+01, Volume fraction 9.6838E-01  Mass fractions:
 FE  9.46531E-01  CR  1.55549E-02  C   3.06184E-03
 NI  2.88106E-02  SI  3.08922E-03  MN  2.95285E-03

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 3.8245E-02, Mass 1.5752E+00, Volume fraction 3.1623E-02  Mass fractions:
 CR  4.94158E-01  C   8.74860E-02  NI  7.42624E-04
 FE  4.13028E-01  MN  4.58537E-03  SI  5.68368E-11

 BCC_A2                      Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.71740E-01  CR  1.04725E-02  MN  8.83251E-04
 NI  1.30178E-02  SI  3.81249E-03  C   7.40352E-05
POLY_3: show tc
   ... the command in full is SHOW_VALUE
 TC=739.45181
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: s-a-v 1 w(c) 0 .08 0.001,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex07 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.550000E-02
...OK

 Phase Region from   0.550000E-02 for:
     BCC_A2
     FCC_A1
     M7C3
 Global check of adding phase at  8.31547E-03
 Calculated     5 equilibria

 Phase Region from   0.831547E-02 for:
     BCC_A2
     CEMENTITE
     FCC_A1
     M7C3
 Global check of removing phase at  1.15396E-02
 Calculated     7 equilibria

 Phase Region from   0.115396E-01 for:
     BCC_A2
     CEMENTITE
     FCC_A1
 Global test at  1.95000E-02 .... OK
 Global check of adding phase at  2.30282E-02
 Calculated    14 equilibria
```

```
 Phase Region from   0.230282E-01 for:
     BCC_A2
     CEMENTITE
     FCC_A1
     GRAPHITE
 Global test at  3.05000E-02 .... OK
 Global test at  4.05000E-02 .... OK
 Global test at  5.05000E-02 .... OK
 Global test at  6.05000E-02 .... OK
 Global test at  7.05000E-02 .... OK
 Global test at  8.00000E-02 .... OK
 Terminating at   0.800000E-01
 Calculated    61 equilibria

 Phase Region from   0.550000E-02 for:
     BCC_A2
     FCC_A1
     M7C3
 Global check of removing phase at  1.56897E-03
 Calculated     6 equilibria

 Phase Region from   0.156897E-02 for:
     BCC_A2
     FCC_A1
 Global test at  1.00115E-15 .... OK
 Terminating at   0.215894E-12
 Calculated     5 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex07\tcex
 07.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x w-p c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y tc
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 7a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: s-s y n 700 800
   ... the command in full is SET_SCALING_STATUS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 7b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex08

```
About
 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex08\tcex08.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of a property diagram for a high speed steel
SYS: @@ i.e. phase fraction plots, activity vs temperature etc.
SYS: @@
SYS: set-log ex08,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: def-dia
   ... the command in full is DEFINE_DIAGRAM
 For binary or ternary diagrams you may prefer the special modules

 You must specify a value for all compositions and the temperature even
 if you want to use it as axis.
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .9 cr 4 mn .3 si .3 w 8 mo 5 v 2
Next alloying element:
Temperature (C) /1000/: 1000
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C   DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 W   DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MO  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 V   DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M6C                      M5C2
 M3C2                     MC_ETA                   MC_SHP
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 Z_PHASE                  FE4N_LP1                 FECN_CHI
 SIGMA                    MU_PHASE                 P_PHASE
 R_PHASE                  CHI_A12                  LAVES_PHASE_C14
 M3SI                     G_PHASE                  CR3SI
 FE2SI                    MSI                      M5SI3
 AL4C3                    FE8SI2C                  SIC

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

 ........................................................

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M6C                      M5C2
 M3C2                     MC_ETA                   MC_SHP
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 Z_PHASE                  FE4N_LP1                 FECN_CHI
 SIGMA                    MU_PHASE                 P_PHASE
 R_PHASE                  CHI_A12                  LAVES_PHASE_C14
 M3SI                     G_PHASE                  CR3SI
 FE2SI                    MSI                      M5SI3
 AL4C3                    FE8SI2C                  SIC

 ........................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
```

```
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

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```

```
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   'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
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   'N. Saunders, COST 507 Report (1998); Cr-Ti'
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   'I. Ansara, unpublished work (1991); Cr-Si'
   'A. Markstrom, Thermo-Calc software AB, 2011'
  -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         31641 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 You must now set an independent axis for your diagram
 as one of the following conditions:
 Condition  1 is temperature (Celsius)
 Condition  2 is mass percent of C
 Condition  3 is mass percent of CR
 Condition  4 is mass percent of MN
 Condition  5 is mass percent of SI
 Condition  6 is mass percent of W
 Condition  7 is mass percent of MO
 Condition  8 is mass percent of V
Give the number of the condition to vary /1/: 1
Minimum value (C) /800/: 600
Maximum value (C) /1800/: 1600

 The second axis can be another of the conditions above and you will then
 calculate a phase diagram.
 Or you may want to plot how some other quantities depend on the selected
 condition and you will then calculate a  "property" diagram.

 In addition to the conditions above you may use these selected
 dependent quantities on the vertical axis:
 Dependent  9 is mass fraction of all phases
 Dependent 10 is composition of a phase
 Dependent 11 is the fraction of a component in all phases
  (In the post processor you may select many other quantities)
Give the number of the quantity on second axis /9/: 9 tcex08 y
 No initial equilibrium, using default
 Step will start from axis value    1273.15
...OK

 Phase Region from    1273.15     for:
     FCC_A1
     FCC_A1#2
     M6C
 Global test at  1.35315E+03 .... OK
 Global test at  1.45315E+03 .... OK
 Global check of removing phase at  1.51799E+03
 Calculated    27 equilibria

 Phase Region from    1517.99     for:
     FCC_A1
     M6C
 Global check of adding phase at  1.51950E+03
 Calculated     3 equilibria

 Phase Region from    1519.50     for:
     LIQUID
     FCC_A1
     M6C
 Global check of adding phase at  1.57015E+03
 Calculated     8 equilibria

 Phase Region from    1570.15     for:
     LIQUID
     BCC_A2
     FCC_A1
     M6C
 Global check of removing phase at  1.57689E+03
 Calculated     4 equilibria

 Phase Region from    1576.89     for:
     LIQUID
     BCC_A2
     FCC_A1
 Global check of removing phase at  1.60196E+03
 Calculated     5 equilibria

 Phase Region from    1601.96     for:
     LIQUID
     BCC_A2
 Global test at  1.67315E+03 .... OK
 Global check of removing phase at  1.69052E+03
 Calculated    12 equilibria

 Phase Region from    1690.52     for:
     LIQUID
 Global test at  1.76315E+03 .... OK
 Global test at  1.86315E+03 .... OK
 Terminating at    1873.15
 Calculated    22 equilibria

 Phase Region from    1273.15     for:
     FCC_A1
     FCC_A1#2
     M6C
 Global test at  1.19315E+03 .... OK
 Global check of adding phase at  1.12656E+03
```
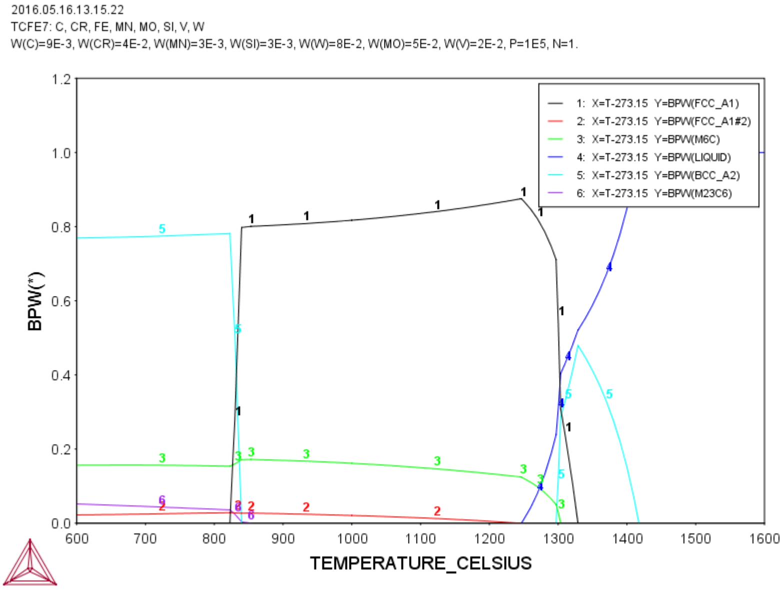
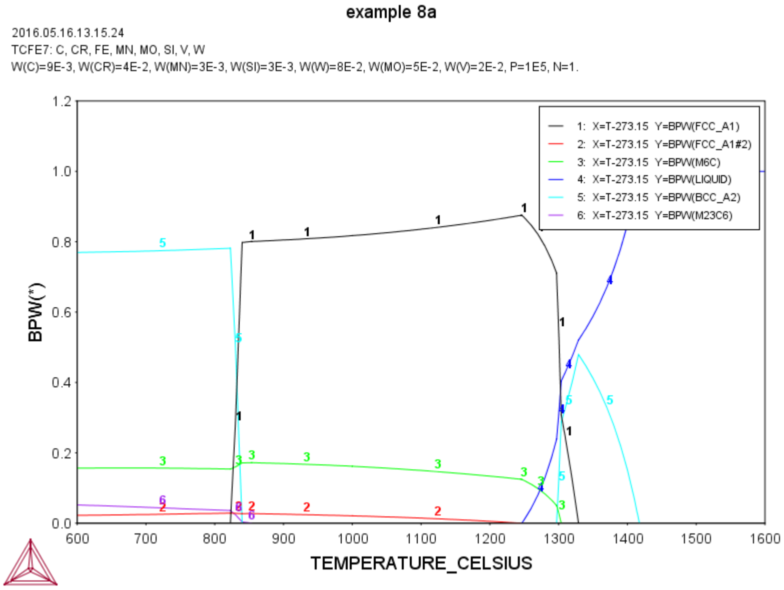

```
Calculated    17 equilibria

Phase Region from    1126.56     for:
    FCC_A1
    FCC_A1#2
    M23C6
    M6C
Global check of adding phase at  1.11294E+03
Calculated     5 equilibria

Phase Region from    1112.94     for:
    BCC_A2
    FCC_A1
    FCC_A1#2
    M23C6
    M6C
Global check of removing phase at  1.09588E+03
Calculated     4 equilibria

Phase Region from    1095.88     for:
    BCC_A2
    FCC_A1#2
    M23C6
    M6C
Global test at  1.02315E+03 .... OK
Global test at  9.23150E+02 .... OK
Terminating at    873.150
Calculated    26 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex08\tcex
08.POLY3

 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes

  ... the command in full is REINITIATE_PLOT_SETTINGS

 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes

  ... the command in full is SET_AUTOMATIC_DIAGRAM_A

Setting automatic diagram axes

  ... the command in full is PLOT_DIAGRAM
```



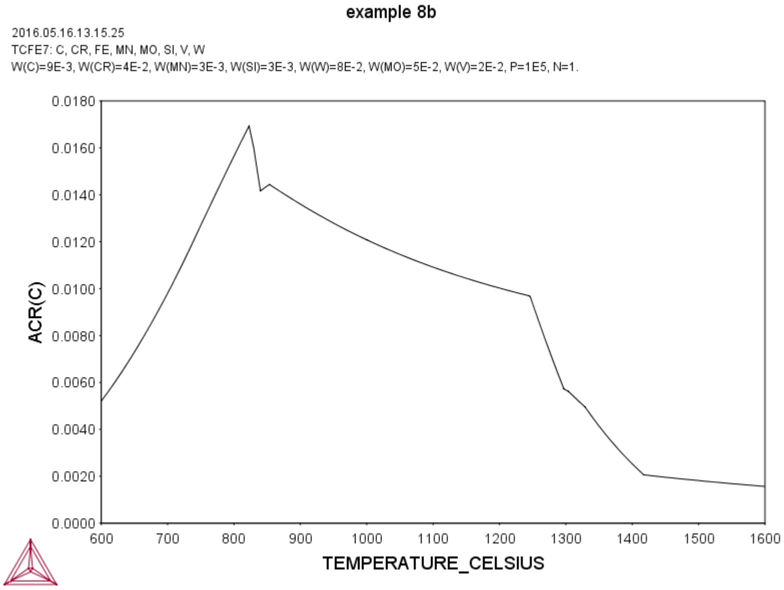
```
POST:
POST:Hit RETURN to continue
POST: set-title example 8a
POST:
POST: plot
  ... the command in full is PLOT_DIAGRAM
```



example 8a

2016.05.16.13.15.24
TCFE7: C, CR, FE, MN, MO, SI, V, W
W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2, W(V)=2E-2, P=1E5, N=1.

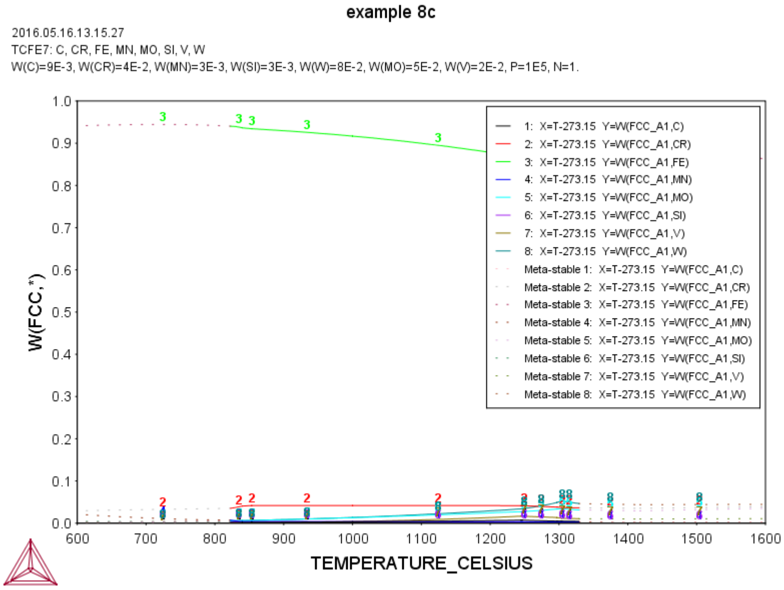
```
POST:
POST:Hit RETURN to continue
POST: s-d-a y acr(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set_lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: n
POST: set-title example 8b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



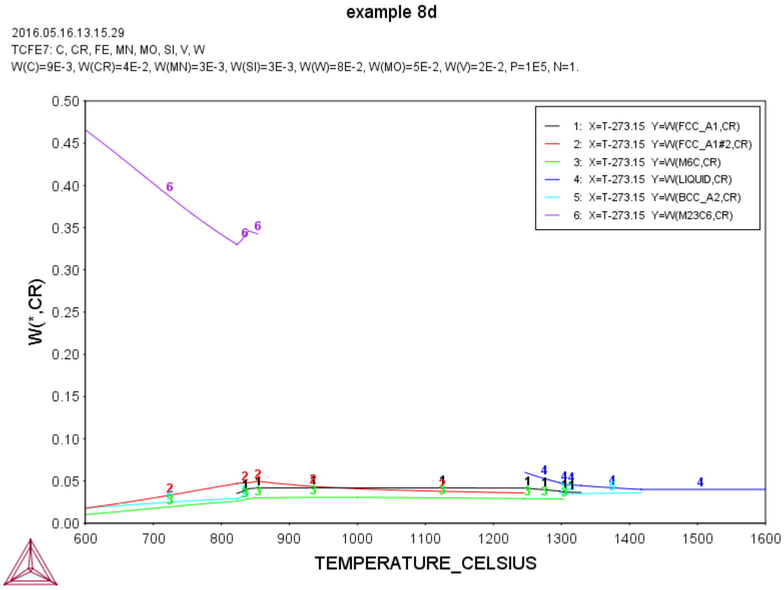
example 8b

2016.05.16.13.15.25
TCFE7: C, CR, FE, MN, MO, SI, V, W
W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2, W(V)=2E-2, P=1E5, N=1.

```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the composition of the austenite (called fcc) varies
POST: @@ Note this is plotted also where the austenite is not stable!
POST: s-d-a y w(fcc,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set_lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 8c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



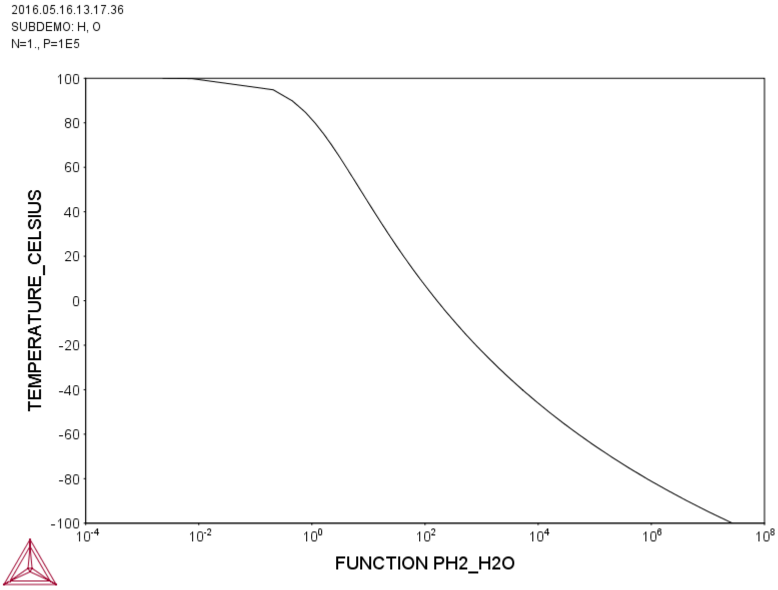
```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the fraction of Cr in all phases
POST: s-d-a y w(*,cr)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 8d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex09

```
About
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex09\tcex09.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of dew point
SYS: @@
SYS:
SYS: go data
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw subdemo
 Current database: Substance Demo Database

 VA                      /-  DEFINED
TDB_SUBDEMO: def-sp h2 h2o1
 H2                      H2O1  DEFINED
TDB_SUBDEMO: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'H2<G> JANAF THERMOCHEMICAL TABLES SGTE ** H2<G> H2<G> HYDROGEN<G>
      STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61'
  'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
  'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
 -OK-
TDB_SUBDEMO: go p-3

 POLY version  3.32
POLY_3: s-c n=1 p=1e5 t=233
POLY_3: ch-st ph h2o_l=f 0
POLY_3: c-e
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           138 grid points in              0 s
    22 ITS,  CPU TIME USED    0 SECONDS
POLY_3: l-e,,,
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 N=1, P=1E5, T=233
 FIXED PHASES
 H2O1_L=0
 DEGREES OF FREEDOM 0

 Temperature    233.00 K (   -40.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00931E+00
 Total Gibbs energy -1.53589E+04,  Enthalpy -9.53654E+02,  Volume  9.68549E-03

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 H                       9.9991E-01  9.9851E-01 3.6499E-04 -1.5335E+04 SER
 O                       9.3929E-05  1.4889E-03 1.0377E-61 -2.7203E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0093E+00, Volume fraction 1.0000E+00  Mass fractions:
 H  9.98511E-01  O  1.48890E-03
 Constitution:
 H2    9.99812E-01  H2O1  1.87875E-04

 H2O1_L                      Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O  8.88103E-01  H  1.11897E-01
POLY_3: ent fun ph2_h2o=acr(h2,gas)/acr(h2o,gas);
POLY_3: s-a-v 1 t 173.15 373.15 ,
POLY_3: save dew y
POLY_3: step normal
 No initial equilibrium, using default
 Step will start from axis value    233.000
...OK

 Phase Region from    233.000     for:
     GAS
     H2O1_L
 Global test at  2.73000E+02 .... OK
 Global test at  3.23000E+02 .... OK
 Global test at  3.73000E+02 .... OK
 Terminating at    373.150
 Calculated    32 equilibria

 Phase Region from    233.000     for:
     GAS
     H2O1_L
 Global test at  1.93000E+02 .... OK
 Terminating at    173.150
 Calculated    15 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex09\dew.
 POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x ph2_h2o
POST: s-a-ty x log
POST: s-d-a y t-c
POST: pl
```



```
POST:
POST:
POST: set-inter
POST:
```

tcex10

About

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex10\tcex10.TCM" set-echo
SYS: @@
SYS: @@ Preventing clogging of Cr2O3
SYS: @@ in a continuous casting process
SYS: @@
SYS: @@ Example showing how to avoid clogging
SYS: @@ in a continuous casting process
SYS: @@
SYS: @@ The background to this example is that a manufacturer wanted
SYS: @@ to increase the Cr content of a material from 18 to 25 weight
SYS: @@ percent. He then had trouble in the continous casting of this
SYS: @@ material because solid Cr2O3 was formed. By calculating the
SYS: @@ equilibria in the steel/slag system a simple correction could
SYS: @@ be found: modify the Mn or Si content, thus decrease the oxygen
SYS: @@ potential.
SYS: @@ In Thermo-calc, one can FIX a phase with zero amount to simulate
SYS: @@ how to avoid forming this phase. One should then release one of the
SYS: @@ conditions, usually one of the compositions, and this composition
SYS: @@ is determined by the equilibrium calculation.
SYS: @@
SYS: set-log ex10,,,,
SYS: @@ The user goes to the database module to obtain data
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: @@ Switch to the database with slag data
TDB_TCFE8: sw slag3
   ... the command in full is SWITCH_DATABASE
 Current database: Fe-containing Slag  v3.2

 FE                      O  DEFINED
 FEOLIQ  REJECTED
TDB_SLAG3: @@ Some information about the database is given by this command
TDB_SLAG3: d-i
   ... the command in full is DATABASE_INFORMATION
 Current database: Fe-containing Slag  v3.2

                SLAG3 -- TCS Fe-containing Slag Database
          *****************************************************
                         (Version 3.2, August, 2012)

      Copyright @ 1992-2012: Thermo-Calc Software, Stockholm, Sweden

   This updated SLAG3 Slag Database contains a liquid SLAG phase, as well
     as an Fe-rich liquid phase (dilute solution), a pure FeO liquid phase,
     a large gaseous mixture phase (with neutral and charged inorganic, as
     well as organic, gaseous species), and many stoichiometric solids and
     solid solution phases (e.g., oxides, silicates, sulfides, halites,
  etc.),
     covering the following 30 elements:
         Ag    Al    Ar    B     C     Ca    Co    Cr    Cu    F
         Fe    H     Mg    Mn    Mo    N     Na    Nb    Ni    O
         P     Pb    S     Si    Sn    Ti    U     V     W     Zr
   Thermodynamic data for the liquid SLAG phase and oxide/silicate solid
     phases in the Al2O3-CaO-CrO-Cr2O3-FeO-Fe2O3-MgO-MnO-Na2O-SiO2-TiO2
     system (with extensions to include sulide/flouride and postulated
     oxide/sulide/flouride/silicate compounds) were critically assessed by
     IRSID (1984) and TCS (since 1997), using the Kapoor-Frohberg-Gaye
     Quasichemical Cell Model, i.e., the Kapoor-Frohberg Slag Model with the
     extensions introduced by Gaye and Welfringer (1984) for complex
     multicomponent liquid slag systems.
   Data for the additional components S and F (as sulfide and fluoride
     species in the framework of [Al+3, Ca+2, Cr+2, Cr+3, Fe+2, Fe+3, Mg+2,
     Mn+2, Na+, Si+4, Ti+4, O-2, S-2 & F-] in the liquid SLAG phase and some
     O-/S-/F-bearing solid slag phases, which were critically assessed by
     IRSID (1997) and TCS (since 1997), have been added to the database,
     and it thus allows calculations of sulfide capacities and many other
     specific properties of liquid SLAG within the framework of 12 elements:
       Al-Ca-Cr-Fe-Mg-Mn-Na-Si-Ti-O-S-F
     More elements and in more redox-states will be gradually included in
     future versions of the SLAG database.
   Note that composition-dependent parameters in various solid solution
     phases have not been considered yet in this particular SLAG3 version,
     implying that at present all the solid phases are simply trated as
     pure/stoiciometric phases. However, it has been planned at TCSAB to
     include complex oxide/silicate/phosphate/sulfide/fluorite/... solid
     solution phases in future versions of the SLAG database.
   Data for a dilute solution of many elements in the Fe-rich liquid phase
     FE_LIQUID are critically assessed and converted to regular solution
     parameters according to Hillert (1986), with modified dilute solution
     parameters (plus a quadratic term) in Fe-rich liquid from Sigworth
     and Elliot (1974), so that it becomes a consistent thermodynamic model
     and also generally improves the agreements of calculated results with
     available experimental data obtained from steel-making metallurgical
     processes. The following 26 dilute components are included in the
     FE_LIQUID solution phase:
       Ag Al B C Ca Co Cr Cu H Mg Mn Mo N Nb Ni O P Pb S Si Sn Ti U V W Zr
     Thermodynamic data for the FE_LIQUID solution phase are evaluated at
     infinite dilution and the recommended composition limit of any minority
     component, in the 27-component diluted Fe-rich liquid, is only 0.1wt%.
     In some cases, data could be used at much higher concentrations in the
     Fe-rich liquid phase (i.e., liquid steel), but the user must carefully
     check each of such cases.
   The SLAG3 database is suitable and efficient for various equilibrium
     calculations of activities, phase equilibria, phase diagrams and
     many other properties in a wide range of metallurgical slag systems,
     especially for (but not limited to) steel-making processes. It can
     be used not only for slag system (liquid slag and solid slag phases)
     but also for alloy-slag-gas heterogeneous interaction processes.
   For steels and various alloys, as well as other substances or solution
     phases, which are in interactions with the Fe-rich FE_LQIUID phase or
     the liquid SLAG phase, thermodynamic data can be appended from other
     available databases, such as TCFE, TCNI, SSOL+SSUB, SALT, TCMP, TCES,
     TTAL/MG/NI/TI, TCAQ, AQS, GCE, NUMT, NUOX, etc. For more information
```

```
     on such databases, please consult Thermo-Calc Software.
   Release History:   Version 1.0 initial release,          1992
                      Version 1.1 with minor improvements,  1998
                      Version 2.0 with major improvements,  2002
                      Version 2.1 with major improvements,  2003
                      Version 2.2 with minor improvements,  2006
                      Version 2.3 adding Ti-species/phases, 2006
                      Version 2.4 with minor improvements,  2008
                      Version 3.0 with major improvements,  2009
                      Version 3.1 with major improvements,  2010
                      Version 3.2 with minor improvements,  2012
   Edited by: Pingfang Shi (Thermo-Calc Software, Sweden), 2002-2010.
              Lina Kjellqvist (Thermo-Calc Software, Sweden), 2012.

TDB_SLAG3:Hit RETURN to continue
TDB_SLAG3: @@ The user defines his system by giving the elements. Note that Fe
TDB_SLAG3: @@ and O are included by default.
TDB_SLAG3: d-sys mn si cr al
   ... the command in full is DEFINE_SYSTEM
 MN                       SI                       CR
 AL  DEFINED
TDB_SLAG3: @@ 'GET' reads thermodynamic data from the database files to the
TDB_SLAG3: @@ program
TDB_SLAG3: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'SLAG2 (2006): TCS Fe-Containing Slag Database, V2.3, owned and provided
      by Thermo-Calc Software.'
  'TCMP2 (2009): TCS Materials Processing Database, V2.5, owned and provided
      by Thermo-Calc Software.'
  'Pingfang Shi (2006), unpublished assessments of CrO/Cr2O3-bearing
      systems. '
  'Lina Kjellqvist (2012), unpublished assessments of Al2O3-SiO2 quasi
      -binary system'
  'L Kjellqvist (2005), unpublished assessments of TiO2-bearing quasi-binary
      systems: Al2O3-TiO2, CaO-TiO2, MgO-TiO2, FeO-TiO2, Fe2O3-TiO2.'
  'Pingfang Shi (2009), unpublished assessments of Fe3O4-bearing systems. '
  'Pingfang Shi (2006), unpublished assessments of SiO2-bearing systems. '
 -OK-
TDB_SLAG3: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ There are many commands in the POLY-3 module
POLY_3: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  EXIT                     REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE              SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                     SELECT_EQUILIBRIUM
 BACK                     INFORMATION              SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE       SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS          SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM         SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA  SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS              SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS             SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN          SET_START_VALUE
 DELETE_SYMBOL            MAP                      SHOW_VALUE
 ENTER_SYMBOL             POST                     STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES          TABULATE
POLY_3:Hit RETURN to continue
POLY_3: @@ Some basic information is given by the INFORMATION command
POLY_3: @@ Look at example 1 for more details.
POLY_3: info
   ... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/: ?

 WHICH SUBJECT

 Specify a subject (or its abbreviation as long as it is unique, e.g.,
 SIN, SIT, SOL, SPE, STATE, STEP, SYM, SYS, SUB, etc.) on which information
 should be given, from the following subjects that are important to the use
 of the POLY module:

  PURPOSE                 GETTING STARTED          USER INTERFACE
  HELP                    MACRO FACILITY           PRIVATE FILES
  BASIC THERMODYNAMICS    SYSTEM AND PHASES        CONSTITUENTS AND SPECIES
  SUBLATTICES             COMPONENTS               SITE AND MOLE FRACTIONS
  COMPOSITION AND CONSTITUTION                     CONCENTRATION
  STATE VARIABLES         INTENSIVE VARIABLES      EXTENSIVE VARIABLES
  DERIVED VARIABLES       UNITS                    BASIC UNITS
  SYSTEM UNITS            COMPONENT UNITS          PHASE UNITS
  PHASE-COMPONENT UNITS   PHASE-SPECIES UNITS      USER-SPECIFIED UNITS
  SYMBOLS                 REFERENCE STATES         METASTABLE EQUILIBRIUM
  CONDITIONS              AXIS-VARIABLES           SPECIAL OPTIONS
  CALCULATIONS TYPES      SINGLE EQUILIBRIUM       INITIAL EQUILIBRIUM
  STEPPING                SOLIDIFICATION PATH      PARAEQUILIBRIUM AND T0
  MAPPING                 PLOTTING OF DIAGRAMS     GLOBAL MINIMIZATION
  DIAGRAM TYPES           BINARY DIAGRAMS          TERNARY DIAGRAMS
  QUASI-BINARY DIAGRAMS   HIGHER ORDER DIAGRAMS    PROPERTY DIAGRAMS
  POTENTIAL DIAGRAMS      POURBAIX DIAGRAMS        AQUEOUS SOLUTIONS
  ORDER-DISORDER          TROUBLE SHOOTING         FAQ

 If you are using the ED_EXP module (the sub-module of the PARROT module),
 you can also get detailed information of the following subject keywords
 which are relevant to the EX_EXP module:

  EDEXP     for Edit-Experiment Module (ED-EXP)
  EDPOLY    for Performance of POLY Commands in the ED_EXP Module
  EDSPECIAL for Special Commands only available in the ED_EXP Module
  EDPOP     for Other Commands in the Experimental Data (POP or DOP) Files
```

```
WHICH SUBJECT /PURPOSE/:
 PURPOSE

         INTRODUCTION to the Equilibrium Calculation Module (POLY)
        ***********************************************************

 Knowledge of the thermodynamic equilibrium is an important factor for
 understanding properties of materials and processes. With a database of
 thermodynamic model parameters, it is possible to predict such properties
 and also to obtain driving forces for diffusion-controlled phase
 transformations and other dynamic processes.

 With the comprehensive Equilibrium Calculation module, POLY ? it is possible
 to calculate many different kinds of equilibria and diagrams, in particular
 multicomponent phase diagrams. This is thus an important tool in developing
 new materials and processes. The current POLY module is its third version;
 this is why is often referred as POLY_3 in the Thermo-Calc software.

 Different kind of databases can be used with the POLY module, and thus it
 can be used for alloys or ceramic system, as well as gaseous equilibria,
 aqueous solution involved heterogeneous interaction systems. Since TCCN,
 up to 40 elements and 1000 species can be defined into a single system
 (previously 20 elements and 400 species) for equilibrium calculations.

 Great care has been taken to provide the users with the most flexible tool.
 All normal thermodynamic state variables can be used to set as conditions in
 calculating equilibria, and as axes in plotting diagrams. A unique facility
 is to set the composition or any property of an individual phase as a
 condition. Any state variable can be varied along an axis in order to
 generate a diagram. During calculations of a diagram, complete descriptions
 of all calculated equilibria are stored, and in the diagram any state
 variable can be used as axis.

 One of the major improvements since the TCCR/TCW4 software version is that
 the recently-implemented Global Minimization Technique is used to assure
 that the present minimum in an equilibrium calculation is the most stable
 minima for the specified conditions. This new technique, which is based
 on the traditional GEM (Gibbs Energy Minimization) Technique (i.e., the
 ordinary POLY Minimization routines used in previous versions, where
 pre-knowledge of miscibility gaps in involved phases are necessary,
 otherwise, metastable equilibria instead of the stable equilibria may be
 obtained), will ultimately prevent a calculation from reaching an undesired
 metastable or unstable (local) equilibrium in a defined system, and
 automatically detect possible miscibility gap(s) and automatically create
 additional composition sets in a solution phase if needed for handling
 single or multiple miscibility gaps. Therefore it is no longer necessary
 for the user to specify additional composition sets in advance.

 A Direct Global Minimization can be performed on conditions: N, n(comp),
 B, b(comp), w(comp), x(comp), T, and P, but not when combined conditions
 as e.g. w(a)-3*w(b)=1 are used or when an activity or potential condition
 is used. For all other types of conditions where regular minimization
 converges, Indirect Global Minimization, i.e. global test and corrections,
 if necessary, are performed until the lowest minimum is found.

  * Direct Global Minimization: From the mesh of Gibbs energy, find the set
     of grid points that gives the lowest energy solution under the specified
     conditions. This set of grid points provides starting combination of
     phases and their constitutions for regular minimization to find the
     exact equilibrium solution. This solution will be then subject to a
     global test as described below.

  * Indirect Global Minimization: Under certain conditions, direct approach
     is impossible. In this case, regular minimization is performed first
     and then a check is performed in order to see if the found local minimum
     is a global one by checking if all grid points are above the equilibrium
     Gibbs energy plane. If not, then recalculate by including these grid
     points until no grid point is above the equilibrium Gibbs energy plane
     from the previous step.

 The full-scale and full-scope usage of the Global Minimization Technique has
 been extended from for only single-point calculations within TCCR/TCW4 to
 for all types of calculations (of single-points, property diagram stepping
 and phase diagram mapping) within TCCS/TCW5.

 The use of Global Minimization Technique may increase the computation time,
 while it is not an issue at all, thanks for the rapid developments of
 computer hardware nowadays.

  * The main cost in time comes from the calculation of Gibbs energy at each
     grid point generated by properly meshing the composition space for each
     entered phase. In a typical multicomponent system calculation, about
     100MB of RAM memory is needed in storing the mesh of Gibbs energies.

  * An additional (but much smaller) cost in time comes from finding the set
     of grid points in the above mesh that give the lowest energy solution.
     This solution is where POLY starts its ordinary minimization. When POLY
     has found an equilibrium, the equilibrium Gibbs energy surface is
     compared to the mesh to assure that no grid point is below the surface,
     i.e. a global minimization has been reached.

 Global Minimization is now performed by default in single-point or
 stepping or mapping equilibrium calculations, but can of course be
 turned off (and on again by repeating the command-sequence of
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION) by the user for specific purposes.
 This means that truly stable equilibrium should be guaranteed for
 single-points, stepping and mapping calculations.
  * A completely new stepping and mapping procedure that ensures Global
     Minimization everywhere it is critical has been developed and been
     made available in TCCS/TCW5. These newly re-written STEP/MAP routines
     are very important for stepping/mapping calculations in multicomponent
     systems where there are complex miscibility gaps in some phases, and
     it does not require having any ??good?? guess of starting points.
     Therefore, TCCS/TCW5 can automatically handle complex solution phases
     with single or multiple miscibility gaps  [for instance, a solution
     phase that is thermodynamically described as a single phase in a
     Thermo-Calc database, such as FCC, BCC or HCP phases, may be split
     into two or several composition-sets/phases that are presented in
     an equilibrium state as metallic phase(s), carbide(s), nitride(s),
     carbonitride(s), nitrocarbide(s), and so on], and can thus ensure
     the correct and complete phase diagrams and property diagrams in
     multicomponent systems, without bothering staring points.

 Together with the PARROT module, the POLY module is also used for critical
 assessment of experimental data in order to develop thermodynamic databases.
 The POLY module uses the Gibbs Energy System (GES) for modeling and data
```

```
 manipulations of the thermodynamic properties of each phase.

 The following commands are available in the POLY module:
 POLY_3:?
  ADD_INITIAL_EQUILIBRIUM  EXIT                     REINITIATE_MODULE
  ADVANCED_OPTIONS         GOTO_MODULE              SAVE_WORKSPACES
  AMEND_STORED_EQUILIBRIA  HELP                     SELECT_EQUILIBRIUM
  BACK                     INFORMATION              SET_ALL_START_VALUES
  CHANGE_STATUS            LIST_AXIS_VARIABLE       SET_AXIS_VARIABLE
  COMPUTE_EQUILIBRIUM      LIST_CONDITIONS          SET_CONDITION
  COMPUTE_TRANSITION       LIST_EQUILIBRIUM         SET_INPUT_AMOUNTS
  CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA  SET_INTERACTIVE
  DEFINE_COMPONENTS        LIST_STATUS              SET_NUMERICAL_LIMITS
  DEFINE_DIAGRAM           LIST_SYMBOLS             SET_REFERENCE_STATE
  DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
  DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN          SET_START_VALUE
  DELETE_SYMBOL            MAP                      SHOW_VALUE
  ENTER_SYMBOL             POST                     STEP_WITH_OPTIONS
  EVALUATE_FUNCTIONS       READ_WORKSPACES          TABULATE
 POLY_3:

 Note that, since TCCS, the SPECIAL_OPTIONS and SET_MINIMIZAION_OPTIONS
 commands (the later one was introduced in the TCCR version) has been merged
 into the new ADVANCED_OPTIONS command; and the RECOVER_START_VALUES command
 has been removed, due to that is not relevant to the POLY module anymore.

 Revision History of the POLY-Module User's Guide:
 ==================================================
  Mar 1991  First release
                    (Edited by Bo Jansson and Bo Sundman)
  Oct 1993  Second revised release (with version J)
                    (Edited by Bo Jansson and Bo Sundman)
  Oct 1996  Third revised release (with version L)
                    (Edited by Bo Sundman)
  Nov 1998  Fourth revised release (with version M)
                    (Edited by Bo Sundman)
  Jun 2000  Fifth revised and extended release
                    (Edited by Pingfang Shi)
  Nov 2002  Sixth revised and extended release
                    (Edited by Pingfang Shi)
  May 2006  Eighth revised and extended release
                    (Edited by Pingfang Shi)
  Apr 2008  Ninth revised and extended release
                    (Edited by Pingfang Shi)


WHICH SUBJECT:
POLY_3:Hit RETURN to continue
POLY_3: @@ Now set the conditions i.e. the temperature, pressure and
POLY_3: @@ composition. We are interested in the situation at the
POLY_3: @@ outflow of steel
POLY_3: s-c t=1800,p=101325,n=1
   ... the command in full is SET_CONDITION
POLY_3: @@ As conditions one can specify that the steel should have
POLY_3: @@ 18 weight percent of Cr, 0.4 w/o Mn and 0.4 w/o Si
POLY_3: @@ (Note that the overall amount of Cr and Mn is not specified).
POLY_3: s-c w(mn)=.004,w(cr)=.18,w(si)=.004
   ... the command in full is SET_CONDITION
POLY_3: @@ The amount of Al is very small, assume 7 ppm
POLY_3: s-c w(al)=7e-6
   ... the command in full is SET_CONDITION
POLY_3: @@ We will later assume that the oxygen potential is determined
POLY_3: @@ by the equilibrium with liquid slag but initially we assume
POLY_3: @@ there is 100 ppm O
POLY_3: s-c w(o)=1e-4
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6,
    W(O)=1E-4
 DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: @@ Let us check what phases we have
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 SIO2_TRIDYMITE           ENTERED      0.000000E+00    0.000000E+00
 SIO2_QUARTZ              ENTERED      0.000000E+00    0.000000E+00
 SIO2_CRISTOBALITE        ENTERED      0.000000E+00    0.000000E+00
 SIO2_BETA_QUARTZ         ENTERED      0.000000E+00    0.000000E+00
 MNO_SIO2                 ENTERED      0.000000E+00    0.000000E+00
 MNO_AL2O3                ENTERED      0.000000E+00    0.000000E+00
 MNO                      ENTERED      0.000000E+00    0.000000E+00
 MN2O2_SIO2               ENTERED      0.000000E+00    0.000000E+00
 FEO_AL2O3                ENTERED      0.000000E+00    0.000000E+00
 FEO                      ENTERED      0.000000E+00    0.000000E+00
 FE3O4                    ENTERED      0.000000E+00    0.000000E+00
 FE2O3                    ENTERED      0.000000E+00    0.000000E+00
 FE2O2_SIO2               ENTERED      0.000000E+00    0.000000E+00
 CR2O3                    ENTERED      0.000000E+00    0.000000E+00
 AL6O9_SI2O4              ENTERED      0.000000E+00    0.000000E+00
 AL2O3                    ENTERED      0.000000E+00    0.000000E+00
 SLAG                     ENTERED      0.000000E+00    0.000000E+00
 FE_LIQUID                ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
POLY_3: @@ We start by assuming all other phases except FE_LIQUID are suspended
POLY_3: ch-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: ch-st p fe-l=ent 0
   ... the command in full is CHANGE_STATUS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6,
    W(O)=1E-4
 DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: @@ The degree of freedoms is zero and we can make a calculation.
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated             20 grid points in              0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       0 s, total time     0  s
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POLY_3: @@ Now set the suspended phases as dormant
POLY_3: c-st p *s=d
   ... the command in full is CHANGE_STATUS
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated            20 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FE_LIQUID               ENTERED      0.000000E+00    1.000000E+00
 AL2O3                   DORMANT     -4.467190E-03
 AL6O9_SI2O4             DORMANT     -4.414257E-02
 SLAG                    DORMANT     -1.124576E-01
 MNO_AL2O3               DORMANT     -1.635823E-01
 FEO_AL2O3               DORMANT     -3.788023E-01
 SIO2_CRISTOBALITE       DORMANT     -4.217466E-01
 SIO2_TRIDYMITE          DORMANT     -4.221446E-01
 SIO2_BETA_QUARTZ        DORMANT     -4.449541E-01
 SIO2_QUARTZ             DORMANT     -4.449674E-01
 CR2O3                   DORMANT     -4.826177E-01
 DORMANT PHASES WITH DRIVING FORCE LESS THAN   -5.733375E-01
 MNO_SIO2 MN2O2_SIO2 FE2O2_SIO2 MNO FEO FE3O4 FE2O3 GAS
POLY_3:Hit RETURN to continue
POLY_3: @@ If the stable phases do not change in 12 iterations the program
POLY_3: @@ terminates even if the program has not calculated the correct
POLY_3: @@ driving forces for the metastable phases.
POLY_3: @@ You can change that and other things by the command SET-NUMERICAL-LIMITS
POLY_3: @@ We now use that to change the lowest value of a fraction variable.
POLY_3: s-n-l 500 1E-6 1E-12 n
   ... the command in full is SET_NUMERICAL_LIMITS
 LIMITATIONS of the present version of Thermo-Calc
 Max number of elements                        :  40
 Max number of species                         :5000
 Max number of sublattices in a phase          :  10
 Max number of constituents in a phase:        : 200
 Max number of constituents in an ideal phase :5000

POLY_3:Hit RETURN to continue
POLY_3: @@ Calculate once more
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FE_LIQUID               ENTERED      0.000000E+00    1.000000E+00
 AL2O3                   DORMANT     -4.467190E-03
 AL6O9_SI2O4             DORMANT     -4.414257E-02
 SLAG                    DORMANT     -1.124576E-01
 MNO_AL2O3               DORMANT     -1.635823E-01
 FEO_AL2O3               DORMANT     -3.788023E-01
 SIO2_CRISTOBALITE       DORMANT     -4.217466E-01
 SIO2_TRIDYMITE          DORMANT     -4.221446E-01
 SIO2_BETA_QUARTZ        DORMANT     -4.449541E-01
 SIO2_QUARTZ             DORMANT     -4.449674E-01
 CR2O3                   DORMANT     -4.826177E-01
 DORMANT PHASES WITH DRIVING FORCE LESS THAN   -5.733375E-01
 MNO_SIO2 MN2O2_SIO2 FE2O2_SIO2 MNO FEO FE3O4 FE2O3 GAS
POLY_3:Hit RETURN to continue
POLY_3: @@ The driving forces are quite stable.
POLY_3: @@ Now set the slag phase stable and let the program
POLY_3: @@ adjust the amount of oxygen to make it stable
POLY_3: c-st p slag=fix 0
   ... the command in full is CHANGE_STATUS
POLY_3: s-c w(o)
   ... the command in full is SET_CONDITION
Value /1E-04/: none
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6
 FIXED PHASES
 SLAG=0
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           426 grid points in              0 s
    53 ITS,  CPU TIME USED   4 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG3

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6
 FIXED PHASES
 SLAG=0
 DEGREES OF FREEDOM 0

 Temperature   1800.00 K (  1526.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.48777E+01
 Total Gibbs energy -1.12615E+05,  Enthalpy  7.09998E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      1.4237E-05  7.0000E-06 2.0544E-10 -3.3383E+05 SER
 CR                      1.8998E-01  1.8000E-01 5.0820E-04 -1.1351E+05 SER
 FE                      7.9778E-01  8.1187E-01 6.2366E-04 -1.1045E+05 SER
 MN                      3.9956E-03  4.0000E-03 2.3985E-06 -1.9367E+05 SER
 O                       4.1841E-04  1.2198E-04 4.1414E-13 -4.2672E+05 SER
 SI                      7.8159E-03  4.0000E-03 4.4720E-08 -2.5327E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4878E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.11871E-01  SI  4.00000E-03  O   1.21983E-04
 CR  1.80000E-01  MN  4.00000E-03  AL  7.00000E-06
```
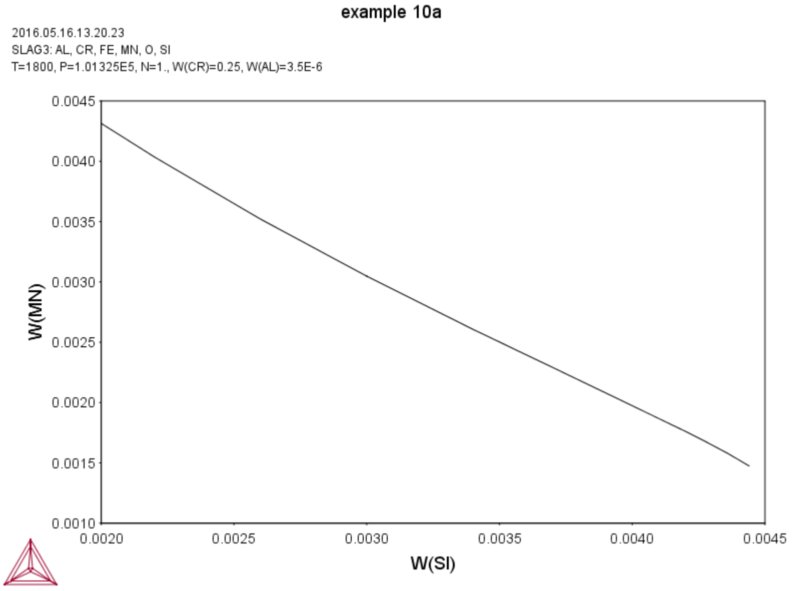

```
 SLAG                          Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   4.10814E-01  MN  1.72313E-01  CR  3.42320E-02
 AL  2.73762E-01  SI  8.14396E-02  FE  2.74396E-02

 AL2O3                         Status DORMANT     Driving force  9.9821E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 AL  5.29261E-01  SI  0.00000E+00  FE  0.00000E+00
 O   4.70739E-01  MN  0.00000E+00  CR  0.00000E+00

 AL6O9_SI2O4                   Status DORMANT     Driving force  6.7904E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   4.88176E-01  SI  1.31839E-01  FE  0.00000E+00
 AL  3.79984E-01  MN  0.00000E+00  CR  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ List also the status of the phases.
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                     STATUS    DRIVING FORCE   MOLES
 SLAG                      FIXED        0.000000E+00    0.000000E+00
 FE_LIQUID                 ENTERED      0.000000E+00    1.000000E+00
 AL2O3                     DORMANT      9.982100E-02
 AL6O9_SI2O4               DORMANT      6.790401E-02
 MNO_AL2O3                 DORMANT     -6.090788E-02
 FEO_AL2O3                 DORMANT     -2.760540E-01
 SIO2_CRISTOBALITE         DORMANT     -2.903040E-01
 SIO2_TRIDYMITE            DORMANT     -2.907021E-01
 SIO2_BETA_QUARTZ          DORMANT     -3.135115E-01
 SIO2_QUARTZ               DORMANT     -3.135249E-01
 CR2O3                     DORMANT     -3.641846E-01
 MNO_SIO2                  DORMANT     -4.550160E-01
 MN2O2_SIO2                DORMANT     -5.626559E-01
 FE2O2_SIO2                DORMANT     -1.244157E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN   -1.355940E+00
 MNO FEO FE3O4 FE2O3 GAS 2
POLY_3:Hit RETURN to continue
POLY_3: @@ Note that mullite and corundum are stable!
POLY_3: @@ The amount of Al is probably too high, set it
POLY_3: @@ to half of the initial value
POLY_3: s-c w(al)=3.5e-6
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    76 ITS,  CPU TIME USED   4 SECONDS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                     STATUS    DRIVING FORCE   MOLES
 SLAG                      FIXED        0.000000E+00    0.000000E+00
 FE_LIQUID                 ENTERED      0.000000E+00    1.000000E+00
 AL6O9_SI2O4               DORMANT      3.462882E-03
 AL2O3                     DORMANT     -5.440445E-02
 SIO2_CRISTOBALITE         DORMANT     -1.302843E-01
 SIO2_TRIDYMITE            DORMANT     -1.306824E-01
 MNO_AL2O3                 DORMANT     -1.367590E-01
 SIO2_BETA_QUARTZ          DORMANT     -1.534919E-01
 SIO2_QUARTZ               DORMANT     -1.535052E-01
 CR2O3                     DORMANT     -2.199493E-01
 MNO_SIO2                  DORMANT     -3.109704E-01
 FEO_AL2O3                 DORMANT     -3.517851E-01
 MN2O2_SIO2                DORMANT     -4.254562E-01
 DORMANT PHASES WITH DRIVING FORCE LESS THAN   -1.106717E+00
 FE2O2_SIO2 MNO FEO FE3O4 FE2O3 GAS F
POLY_3: @@ The Al2O3 phases are now not stable.
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0   , database: SLAG3

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=3.5E-6
 FIXED PHASES
 SLAG=0
 DEGREES OF FREEDOM 0

 Temperature   1800.00 K (  1526.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams   5.48735E+01
 Total Gibbs energy -1.12649E+05,  Enthalpy  7.09791E+04,  Volume  0.00000E+00

 Component                 Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                        7.1180E-06  3.5000E-06 9.7338E-11 -3.4501E+05 SER
 CR                        1.8996E-01  1.8000E-01 5.0779E-04 -1.1352E+05 SER
 FE                        7.9769E-01  8.1184E-01 6.2371E-04 -1.1045E+05 SER
 MN                        3.9953E-03  4.0000E-03 2.3967E-06 -1.9368E+05 SER
 O                         5.3132E-04  1.5491E-04 5.2696E-13 -4.2312E+05 SER
 SI                        7.8153E-03  4.0000E-03 4.4640E-08 -2.5330E+05 SER

 FE_LIQUID                     Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4873E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.11842E-01  MN  4.00000E-03  O   1.54912E-04
 CR  1.80000E-01  SI  4.00000E-03  AL  3.50000E-06

 SLAG                          Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   3.96074E-01  AL  1.63086E-01  CR  4.06215E-02
 MN  2.36807E-01  SI  1.36167E-01  FE  2.72458E-02

 AL6O9_SI2O4                   Status DORMANT     Driving force  3.4629E-03
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   4.88176E-01  SI  1.31839E-01  FE  0.00000E+00
 AL  3.79984E-01  MN  0.00000E+00  CR  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ We assume that this describes the situation at 18 w/o Cr. Some
POLY_3: @@ liquid slag that later will form mainly SiO2-Al2O3-MnO is present.
POLY_3: @@ Now increase the Cr-content to 25 w/o
POLY_3: s-c w(cr)=.25
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
```

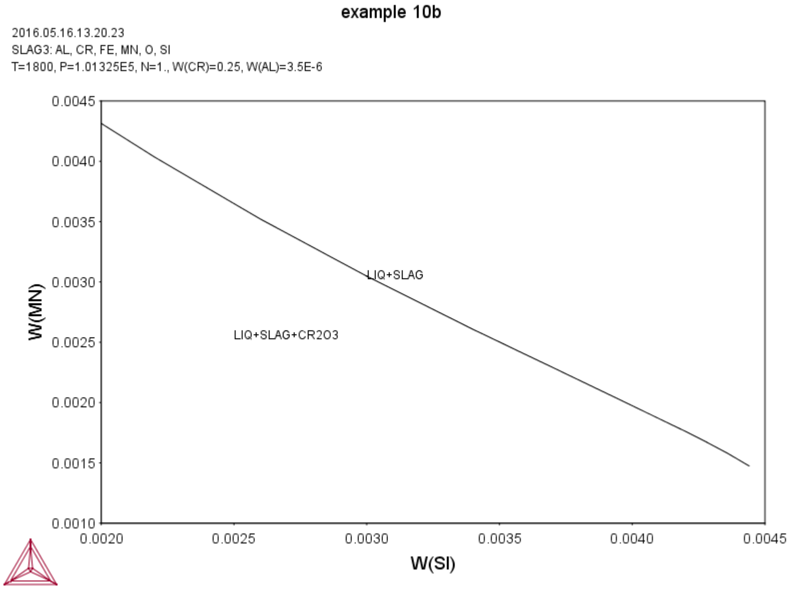
```
 Using already calculated grid
    71 ITS,  CPU TIME USED   4 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG3

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=3.5E-6
 FIXED PHASES
 SLAG=0
 DEGREES OF FREEDOM 0

 Temperature   1800.00 K (  1526.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45773E+01
 Total Gibbs energy -1.12779E+05,  Enthalpy  7.08202E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      7.0796E-06  3.5000E-06 7.7978E-11 -3.4833E+05 SER
 CR                      2.6241E-01  2.5000E-01 6.9368E-04 -1.0886E+05 SER
 FE                      7.2484E-01  7.4171E-01 5.6880E-04 -1.1183E+05 SER
 MN                      3.9737E-03  4.0000E-03 2.5522E-06 -1.9274E+05 SER
 O                       9.9119E-04  2.9056E-04 5.4210E-13 -4.2269E+05 SER
 SI                      7.7732E-03  4.0000E-03 4.4207E-08 -2.5344E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4577E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  7.41706E-01  SI  4.00000E-03  O   2.90561E-04
 CR  2.50000E-01  MN  4.00000E-03  AL  3.50000E-06

 SLAG                        Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   3.85022E-01  SI  1.41920E-01  CR  5.93665E-02
 MN  2.64912E-01  AL  1.25822E-01  FE  2.29577E-02
POLY_3:Hit RETURN to continue
POLY_3: @@ Now Cr2O3 would like to be stable. The simplest correction is to modify
POLY_3: @@ the composition of the steel in order to decrease the oxygen potential.
POLY_3: @@ For example the Mn or Si content could be changed.
POLY_3: @@ In order to determine which of these has the largest influence
POLY_3: @@ on the oxygen potential, calculate this by the partial derivative
POLY_3: @@ of the oxygen activity w.r.t. the Mn and Si content.
POLY_3: s-ref-s o gas
   ... the command in full is SET_REFERENCE_STATE
Temperature /*/:
Pressure /1E5/:
POLY_3: show acr(o)
   ... the command in full is SHOW_VALUE
 ACR(O)=7.9408178E-7
POLY_3: show acr(o).w(mn)
   ... the command in full is SHOW_VALUE
 ACR(O).W(MN)=-4.6033449E-5
POLY_3: show acr(o).w(si)
   ... the command in full is SHOW_VALUE
 ACR(O).W(SI)=-5.2536001E-5
POLY_3:Hit RETURN to continue
POLY_3: @@ The value is largest for Si and thus the smallest change is necessary
POLY_3: @@ for that. Instead of modifying this content in steps one may
POLY_3: @@ specify that the Cr2O3 phase should be on its limit of stability, i.e.
POLY_3: @@ set it FIX with zero amount and calculate the change in composition.
POLY_3: c-s p cr2o3=fix 0
   ... the command in full is CHANGE_STATUS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=3.5E-6
 FIXED PHASES
 SLAG=0           CR2O3=0
 DEGREES OF FREEDOM -1
POLY_3: s-c w(si)=none
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           427 grid points in              0 s
    75 ITS,  CPU TIME USED   4 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG3

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(AL)=3.5E-6
 FIXED PHASES
 SLAG=0           CR2O3=0
 DEGREES OF FREEDOM 0

 Temperature   1800.00 K (  1526.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.46679E+01
 Total Gibbs energy -1.12301E+05,  Enthalpy  7.11953E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      7.0913E-06  3.5000E-06 7.3390E-11 -3.4924E+05 SER
 CR                      2.6285E-01  2.5000E-01 6.9469E-04 -1.0883E+05 SER
 FE                      7.2776E-01  7.4346E-01 5.7139E-04 -1.1176E+05 SER
 MN                      3.9803E-03  4.0000E-03 2.4897E-06 -1.9311E+05 SER
 O                       1.0707E-03  3.1335E-04 9.0372E-07 -2.0828E+05 GAS
 SI                      4.3351E-03  2.2271E-03 2.3558E-08 -2.6286E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4668E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  7.43456E-01  MN  4.00000E-03  O   3.13352E-04
 CR  2.50000E-01  SI  2.22708E-03  AL  3.50000E-06

 SLAG                        Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   3.71218E-01  AL  1.53107E-01  CR  9.41709E-02
 MN  2.62012E-01  SI  9.43792E-02  FE  2.51128E-02

 CR2O3                       Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CR  6.84207E-01  AL  0.00000E+00  FE  0.00000E+00
 O   3.15793E-01  MN  0.00000E+00  SI  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ We can read the new Si content from this list but also
```

```
POLY_3: @@ show the value of a variable directly
POLY_3: sh w(si)
   ... the command in full is SHOW_VALUE
 W(SI)=2.2270814E-3
POLY_3: @@ We have to increase the Si content to 0.4 w/o to avoid
POLY_3: @@ forming Cr2O3. Calculate also how much the Mn content must be changed
POLY_3: s-c w(si)=.004
   ... the command in full is SET_CONDITION
POLY_3: s-c w(mn)=none
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
   104 ITS,  CPU TIME USED   6 SECONDS
POLY_3: sh w(mn)
   ... the command in full is SHOW_VALUE
 W(MN)=1.9763402E-3
POLY_3: @@ Check with Si content equal to 0.3. It should be consistent with
POLY_3: @@ the plot below, i.e. Mn content decreases with increasing Si content.
POLY_3: s-c w(si)=.003
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    78 ITS,  CPU TIME USED   5 SECONDS
POLY_3: sh w(mn)
   ... the command in full is SHOW_VALUE
 W(MN)=3.0479009E-3
POLY_3:Hit RETURN to continue
POLY_3: @@ Plot how the Mn content varies when the Si content
POLY_3: @@ varies between 0.2 and 0.8 w/o.
POLY_3: s-a-v 1 w(si) 0.002 0.008 0.0004
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex10 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.300000E-02
...OK

 Phase Region from   0.300000E-02 for:
     FE_LIQUID
     SLAG
     CR2O3
 QBSMER trying to find equilibrium at   4.5200000E-03
 QBSMER: Second global calculation
 Calculated     9 equilibria
 Sorry cannot continue  1717  55 1    4.4400000E-03

 Phase Region from   0.300000E-02 for:
     FE_LIQUID
     SLAG
     CR2O3
 Terminating at   0.200000E-02
 Calculated     6 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex10\tcex
 10.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x w(si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(mn)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 10a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:Hit RETURN to continue
POST: add .003 .003 n
   ... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG
Text size: /.36/:
POST: add .0025 .0025 n
   ... the command in full is ADD_LABEL_TEXT
```

```
Text: LIQ+SLAG+CR2O3
Text size: /.36/:
POST: set-title example 10b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex11

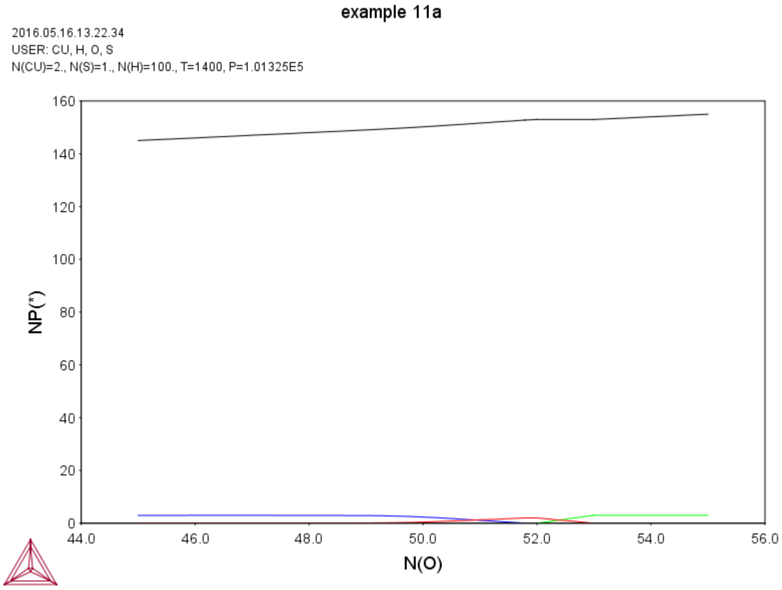
```
About License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex11\tcex11.TCM" set-echo
SYS: @@
SYS: @@ Oxidation of Cu2S with H2O/O2 gas
SYS: @@
SYS: @@ Oxidation of Cu2S with H2O and O2 gas mixture
SYS: @@   Different O/H ratio represents different oxygen potential. Certain
SYS: @@   oxygen potential can desulphurize Cu2S without forming copper oxides.
SYS: @@   This example demonstrates how to find the optimum O/H ratio (i.e. oxygen
SYS: @@   potential).
SYS: @@   In Thermo-calc, the problem reduces to perform equilibria calculations in
SYS: @@   Cu-S-H-O system. The amounts of the components should be kept to correct
SYS: @@   ratio corresponding to Cu2S and H2O, by using a command SET_INPUT_
SYS: @@   AMOUNTS in POLY_3. Initially, O/H = 0.5 is given. Optimum O/H ratio
SYS: @@   is calculated by giving desired calculation conditions. For example,
SYS: @@   to simulate one phase disappearing, one can FIX the phase with zero amount
SYS: @@   in Thermo-calc.
SYS: @@
SYS: set-log ex11,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw
   ... the command in full is SWITCH_DATABASE
 Use one of these databases

 TCFE8   =  Steels/Fe-Alloys  v8.0
 TCFE9   =  Steels/Fe-Alloys  v9.0 SNAPSHOT
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 TCNI8   =  Ni-Alloys  v8.0
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.0
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.0 SNAPSHOT
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0 SNAPSHOT
 TCCU1   =  Copper  v1.0 SNAPSHOT
 TCCC1   =  Cemented carbide  v1.0
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9f
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB5   =  SGTE Substances Database v5.1
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Nobel Metal Alloys Database v3.1
 SNOB2   =  SGTE Nobel Metal Alloys Database v2.1
 SNOB1   =  SGTE Nobel Metal Alloys Database v1.2
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SNUX6   =  SGTE In-Vessel Nuclear Oxide TDB v6.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.0 snapshot
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0 SNAPSHOT
 TCOX6   =  Metal Oxide Solutions  v6.1
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCSLD3  =  Solder Alloys  v3.1
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.0
 TCSI1   =  Ultrapure Silicon  v1.1
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUTO1   =  U-Zr-Si Ternary Oxides TDB v1.1
 NUTA1   =  Ag-Cd-In Ternary Alloys TDB v1.1
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11
 TCAQ2   =  Aqueous Solution  v2.5
 AQS2    =  TGG Aqueous Solution Database v2.5
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
```

```
 ALDEMO  =  Aluminum Demo Database
 FEDEMO  =  Iron Demo Database
 NIDEMO  =  Nickel Demo Database
 SLDEMO  =  Solder Demo Database
 OXDEMO  =  Oxide Demo Database
 SUBDEMO =  Substance Demo Database
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 MOB2    =  Alloys Mobility  v2.4
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0 SNAPSHOT
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database
 MFEDEMO =  Fe-Alloys Mobility demo database
 MNIDEMO =  Ni-Alloys Mobility demo database
 USER    =  User defined Database

DATABASE NAME /TCFE8/: user tcex11.tdb
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                       /-  DEFINED
TDB_USER: def-sys cu s o h
   ... the command in full is DEFINE_SYSTEM
 CU                       S                        O
 H  DEFINED
TDB_USER: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 GAS:G        :CU CU1H1 CU1H1O1 CU1O1 CU1S1 CU2 CU2S1 H H1O1 H1O1S1_HSO
  H1O1S1_SOH H1O2 H1S1 H2 H2O1 H2O1S1_H2SO H2O1S1_HSOH H2O2 H2O4S1 H2S1 H2S2
  O O1S1 O1S2 O2 O2S1 O3 O3S1 S S2 S3 S4 S5 S6 S7 S8:
 CU           :CU:
 CU2O         :CU2O1:
 CU2O_L       :CU2O1:
 CU2S         :CU2S1:
 CU2SO4       :CU2O4S1:
 CU2SO5       :CU2O5S1:
 CU2S_L       :CU2S1:
 CU2S_S2      :CU2S1:
 CU2S_S3      :CU2S1:
 CUO          :CU1O1:
 CUS          :CU1S1:
 CUSO4        :CU1O4S1:
 CU_L         :CU:
 H2O2_L       :H2O2:
 H2O_L        :H2O1:
 H2SO4_L      :H2O4S1:
 S            :S:
 S_L          :S:
 S_S2         :S:
TDB_USER:Hit RETURN to continue
TDB_USER: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous species, stoichiometric solids and
      liquids in the Cu-Fe-H-N-O-S system.'
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  EXIT                     REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE              SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                     SELECT_EQUILIBRIUM
 BACK                     INFORMATION              SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE       SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS          SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM         SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA  SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS              SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS             SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN          SET_START_VALUE
 DELETE_SYMBOL            MAP                      SHOW_VALUE
 ENTER_SYMBOL             POST                     STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES          TABULATE
POLY_3: li-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 CU                       ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 S                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 S_S2                     ENTERED      0.000000E+00    0.000000E+00
 S_L                      ENTERED      0.000000E+00    0.000000E+00
 S                        ENTERED      0.000000E+00    0.000000E+00
 H2SO4_L                  ENTERED      0.000000E+00    0.000000E+00
```

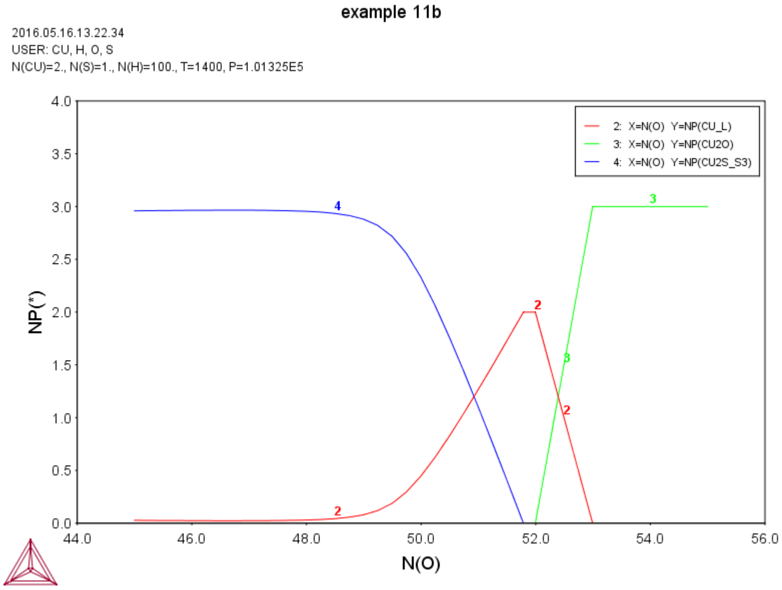
```
 H2O_L                  ENTERED      0.000000E+00    0.000000E+00
 H2O2_L                 ENTERED      0.000000E+00    0.000000E+00
 CU_L                   ENTERED      0.000000E+00    0.000000E+00
 CUSO4                  ENTERED      0.000000E+00    0.000000E+00
 CUS                    ENTERED      0.000000E+00    0.000000E+00
 CUO                    ENTERED      0.000000E+00    0.000000E+00
 CU2S_S3                ENTERED      0.000000E+00    0.000000E+00
 CU2S_S2                ENTERED      0.000000E+00    0.000000E+00
 CU2S_L                 ENTERED      0.000000E+00    0.000000E+00
 CU2SO5                 ENTERED      0.000000E+00    0.000000E+00
 CU2SO4                 ENTERED      0.000000E+00    0.000000E+00
 CU2S                   ENTERED      0.000000E+00    0.000000E+00
 CU2O_L                 ENTERED      0.000000E+00    0.000000E+00
 CU2O                   ENTERED      0.000000E+00    0.000000E+00
 CU                     ENTERED      0.000000E+00    0.000000E+00
 GAS                    ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CU          ENTERED    H15O10.5S1  ENTERED    O           ENTERED
 CU1H1       ENTERED    H1O1        ENTERED    O1S1        ENTERED
 CU1H10O9S1  ENTERED    H1O1S1_HSO  ENTERED    O1S2        ENTERED
 CU1H1O1     ENTERED    H1O1S1_SOH  ENTERED    O2          ENTERED
 CU1H2O2     ENTERED    H1O2        ENTERED    O2S1        ENTERED
 CU1H2O5S1   ENTERED    H1S1        ENTERED    O3          ENTERED
 CU1H6O7S1   ENTERED    H2          ENTERED    O3S1        ENTERED
 CU1O1       ENTERED    H2O1        ENTERED    S           ENTERED
 CU1O4S1     ENTERED    H2O1S1_H2SO ENTERED    S2          ENTERED
 CU1S1       ENTERED    H2O1S1_HSOH ENTERED    S3          ENTERED
 CU2         ENTERED    H2O2        ENTERED    S4          ENTERED
 CU2O1       ENTERED    H2O4S1      ENTERED    S5          ENTERED
 CU2O4S1     ENTERED    H2S1        ENTERED    S6          ENTERED
 CU2O5S1     ENTERED    H2S2        ENTERED    S7          ENTERED
 CU2S1       ENTERED    H4O5S1      ENTERED    S8          ENTERED
 H           ENTERED    H6O6S1      ENTERED    VA          ENTERED
 H10O8S1     ENTERED    H8O7S1      ENTERED
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ Assume initially that we have one mole of Cu2S and 50 moles water vapor
POLY_3: s-i-a n(cu2s1)=1,n(h2o1)=50
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: set-cond t=1400,p=101325
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           685 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
 DEGREES OF FREEDOM 0

 Temperature   1400.00 K (  1126.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.53000E+02,  Mass in grams  1.05989E+03
 Total Gibbs energy -2.75931E+07,  Enthalpy -9.82382E+06,  Volume  5.76972E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CU                      2.0000E+00  1.1991E-01 1.6098E-03 -7.4867E+04 SER
 H                       1.0000E+02  9.5095E-02 9.5714E-06 -1.3452E+05 SER
 O                       5.0000E+01  7.5475E-01 5.1729E-11 -2.7570E+05 SER
 S                       1.0000E+00  3.0248E-02 2.0746E-08 -2.0593E+05 SER

 GAS                            Status ENTERED     Driving force  0.0000E+00
 Moles 1.5022E+02, Mass 9.0794E+02, Volume fraction 1.0000E+00  Mass fractions:
 O   8.81060E-01  H   1.11009E-01  S   7.92556E-03  CU  5.01241E-06
 Constitution:
 H2O1         9.86660E-01  CU1H1O1      1.96753E-08  CU1O1        8.58177E-12
 H2           8.86811E-03  O3S1         1.43507E-08  H2O2         5.46461E-12
 O2S1         4.44169E-03  H2O1S1_HSOH  7.52014E-09  H2O1S1_H2SO  3.12748E-12
 H2S1         2.10471E-05  S            4.30477E-09  H2O4S1       3.10120E-12
 O1S1         5.63051E-06  O2           2.46248E-09  S3           1.29650E-12
 CU           1.32327E-06  H1O1S1_SOH   1.77241E-09  H1O2         4.13438E-13
 H1O1         1.00104E-06  CU1S1        1.23642E-09  S4           3.25596E-18
 H            4.55656E-07  CU2          4.47851E-10  S5           1.21560E-21
 H1S1         3.40802E-07  CU2S1        2.11636E-10  O3           1.70006E-22
 S2           1.38936E-07  H2S2         1.77731E-10  S6           5.54892E-27
 CU1H1        8.04525E-08  O            4.66615E-11  S8           1.00000E-30
 O1S2         2.49875E-08  H1O1S1_HSO   3.35706E-11  S7           1.00000E-30

 CU2S_S3                        Status ENTERED     Driving force  0.0000E+00
 Moles 2.3266E+00, Mass 1.2343E+02, Volume fraction 0.0000E+00  Mass fractions:
 CU  7.98557E-01  S   2.01443E-01  O   0.00000E+00  H   0.00000E+00

 CU_L                           Status ENTERED     Driving force  0.0000E+00
 Moles 4.4883E-01, Mass 2.8522E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  1.00000E+00  S   0.00000E+00  O   0.00000E+00  H   0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Now set the status of the diginite (CU2S_S3) to be fixed with
POLY_3: @@ zero amount. This means that we will reduce this completely
POLY_3: c-s
   ... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): cu2s_s3
Status: /ENTERED/: fix
Number of moles /0/: 0
POLY_3: @@ We have now too many conditions as we must allow the gas to vary
POLY_3: @@ in composition to find the correct oxygen potential
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
 FIXED PHASES
 CU2S_S3=0
 DEGREES OF FREEDOM -1
POLY_3:Hit RETURN to continue
POLY_3: set-c n(o)=none
   ... the command in full is SET_CONDITION
```

```
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
 FIXED PHASES
 CU2S_S3=0
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           685 grid points in             0 s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
 FIXED PHASES
 CU2S_S3=0
 DEGREES OF FREEDOM 0

 Temperature   1400.00 K (  1126.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.54785E+02,  Mass in grams  1.08845E+03
 Total Gibbs energy -2.80759E+07,  Enthalpy -1.00131E+07,  Volume  5.85888E+00

 Component               Moles      W-Fraction  Activity   Potential  Ref.stat
 CU                      2.0000E+00  1.1676E-01 1.6098E-03 -7.4867E+04 SER
 H                       1.0000E+02  9.2600E-02 6.5700E-06 -1.3890E+05 SER
 O                       5.1785E+01  7.6118E-01 1.0863E-10 -2.6707E+05 SER
 S                       1.0000E+00  2.9455E-02 2.0746E-08 -2.0593E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.5278E+02, Mass 9.6136E+02, Volume fraction 1.0000E+00  Mass fractions:
 O   8.61805E-01  H   1.04841E-01  S   3.33486E-02  CU  4.75131E-06
 Constitution:
 H2O1         9.76211E-01  O1S2         5.24705E-08  H2O4S1       2.84109E-11
 O2S1         1.95855E-02  CU1H1O1      2.83599E-08  CU1O1        1.80206E-11
 H2           4.17844E-03  O2           1.08582E-08  H2O2         1.13535E-11
 O1S1         1.18234E-05  H2O1S1_HSOH  7.44050E-09  H2O1S1_H2SO  3.09435E-12
 H2S1         9.91688E-06  S            4.30477E-09  S3           1.29650E-12
 H1O1         1.44290E-06  H1O1S1_SOH   2.55475E-09  H1O2         1.25138E-12
 CU           1.32327E-06  CU1S1        1.23642E-09  S4           3.25596E-18
 H            3.12773E-07  CU2          4.47851E-10  O3           1.57414E-21
 H1S1         2.33934E-07  CU2S1        2.11636E-10  S5           1.21560E-21
 S2           1.38936E-07  O            9.79832E-11  S6           5.54892E-27
 O3S1         1.32878E-07  H2S2         8.37427E-11  S8           1.00000E-30
 CU1H1        5.52244E-08  H1O1S1_HSO   4.83886E-11  S7           1.00000E-30

 CU_L                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00  Mass fractions:
 CU  1.00000E+00  S   0.00000E+00  O   0.00000E+00  H   0.00000E+00

 CU2S_S3                     Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CU  7.98557E-01  S   2.01443E-01  O   0.00000E+00  H   0.00000E+00
POLY_3: sh n(*)
   ... the command in full is SHOW_VALUE
 N(CU)=2, N(H)=100., N(O)=51.784749, N(S)=1.
POLY_3:Hit RETURN to continue
POLY_3: @@ If we have too much oxygen we may get some copper oxides,
POLY_3: @@ check which one is the closest to be stable
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 CU2S_S3                 FIXED        0.000000E+00    0.000000E+00
 CU_L                    ENTERED      0.000000E+00    1.999928E+00
 GAS                     ENTERED      0.000000E+00    1.527848E+02
 CU2S_L                  ENTERED     -3.931114E-04    0.000000E+00
 CU2S_S2                 ENTERED     -3.309936E-02    0.000000E+00
 CU                      ENTERED     -3.549960E-02    0.000000E+00
 CU2S                    ENTERED     -3.332974E-01    0.000000E+00
 CU2O                    ENTERED     -1.086153E+00    0.000000E+00
 CU2O_L                  ENTERED     -1.231036E+00    0.000000E+00
 H2O_L                   ENTERED     -1.738865E+00    0.000000E+00
 CUS                     ENTERED     -3.173417E+00    0.000000E+00
 CUO                     ENTERED     -3.229722E+00    0.000000E+00
 CU2SO4                  ENTERED     -3.322206E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -3.797595E+00
 CU2SO5 CUSO4 H2SO4_L H2O2_L S_L S_S2 S
POLY_3: @@ Set Cu2O to fix with zero amount and remove the fix status of CU2S_S3
POLY_3: c-s p cu2o=fix 0
   ... the command in full is CHANGE_STATUS
POLY_3: c-s p cu2s_s3
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           685 grid points in             0 s
    39 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
 FIXED PHASES
 CU2O=0
 DEGREES OF FREEDOM 0

 Temperature   1400.00 K (  1126.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.54993E+02,  Mass in grams  1.09178E+03
 Total Gibbs energy -2.81294E+07,  Enthalpy -1.00609E+07,  Volume  5.85900E+00

 Component               Moles      W-Fraction  Activity   Potential  Ref.stat
 CU                      2.0000E+00  1.1641E-01 1.6098E-03 -7.4867E+04 SER
 H                       1.0000E+02  9.2317E-02 1.2909E-06 -1.5784E+05 SER
 O                       5.1993E+01  7.6191E-01 2.8253E-09 -2.2914E+05 SER
 S                       1.0000E+00  2.9365E-02 3.0696E-11 -2.8178E+05 SER
```

```
 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.5299E+02, Mass 9.6469E+02, Volume fraction 1.0000E+00  Mass fractions:
 O   8.62282E-01  H   1.04479E-01  S   3.32335E-02  CU  4.97350E-06
 Constitution:
 H2O1         9.80215E-01  H2O4S1       7.42671E-10  H1O1S1_HSO   3.65881E-13
 O2S1         1.96037E-02  H2S1         5.66454E-10  CU2S1        3.13135E-13
 H2           1.61310E-04  CU1O1        4.68706E-10  S2           3.04157E-13
 H1O1         7.37378E-06  CU2          4.47851E-10  H2O1S1_H2SO  4.59716E-15
 O2           7.34547E-06  H2O2         2.96508E-10  O3           2.76971E-17
 O3S1         3.45929E-06  H1O2         1.66331E-10  H2S2         7.07748E-18
 CU           1.32327E-06  H1S1         6.80080E-11  S3           4.19951E-21
 O1S1         4.55002E-07  H1O1S1_SOH   1.93172E-11  S4           1.56044E-29
 CU1H1O1      1.44930E-07  H2O1S1_HSOH  1.10541E-11  S7           1.00000E-30
 H            6.14543E-08  S            6.36932E-12  S5           1.00000E-30
 CU1H1        1.08506E-08  O1S2         2.98765E-12  S6           1.00000E-30
 O            2.54848E-09  CU1S1        1.82939E-12  S8           1.00000E-30

 CU_L                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00  Mass fractions:
 CU  1.00000E+00  S   0.00000E+00  O   0.00000E+00  H   0.00000E+00

 CU2O                        Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CU  8.88190E-01  O   1.11810E-01  S   0.00000E+00  H   0.00000E+00
POLY_3: show n(*)
   ... the command in full is SHOW_VALUE
 N(CU)=2, N(H)=100., N(O)=51.992866, N(S)=1.
POLY_3:Hit RETURN to continue
POLY_3: @@ The ratio N(O) to N(H) should thus be between 0.5178 and 0.52
POLY_3: @@ in order to reduce all Cu2S and not forming any Cu2O
POLY_3: @@ Make a diagram showing this amounts of phases
POLY_3: c-st p cu2o
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: s-a-v 1 n(o)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 45
Max value /1/: 55
Increment /.25/:
POLY_3: s-c n(o)
   ... the command in full is SET_CONDITION
Value /51.99286556/:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           685 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0   s
POLY_3: save tcex11 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    51.9929
...OK

 Phase Region from    51.9929     for:
     GAS
     CU_L
 Global check of adding phase at  5.19929E+01
 Calculated     2 equilibria

 Phase Region from    51.9929     for:
     GAS
     CU2O
     CU_L
 Global check of removing phase at  5.29928E+01
 Calculated     6 equilibria

 Phase Region from    52.9928     for:
     GAS
     CU2O
 Global test at  5.49929E+01 .... OK
 Terminating at    55.0000
 Calculated    12 equilibria

 Phase Region from    51.9929     for:
     GAS
     CU_L
 Global check of adding phase at  5.17847E+01
 Calculated     3 equilibria

 Phase Region from    51.7847     for:
     GAS
     CU2S_S3
     CU_L
 Global test at  4.99929E+01 .... OK
 Global test at  4.74929E+01 .... OK
 Global test at  4.50000E+01 .... OK
 Terminating at    45.0000
 Calculated    31 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex11\tcex
 11.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 11a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s y n 0 4
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 11b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



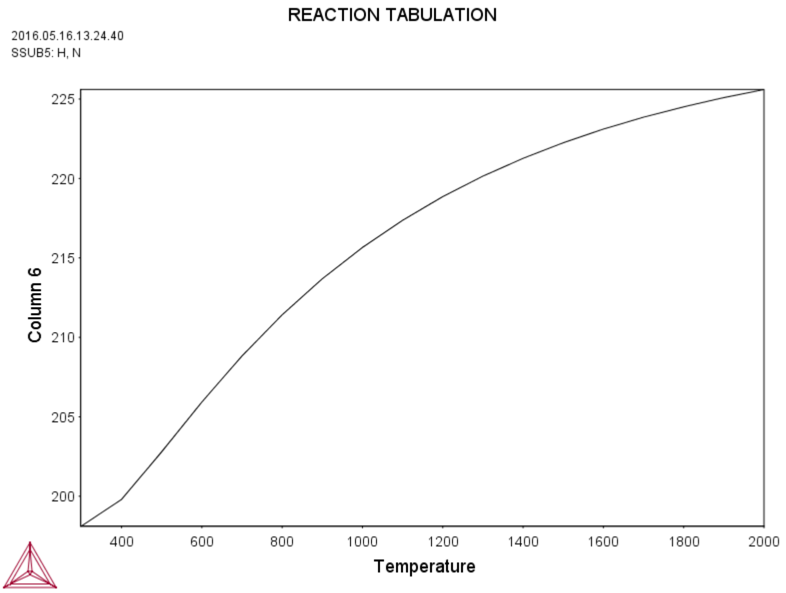
```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex12

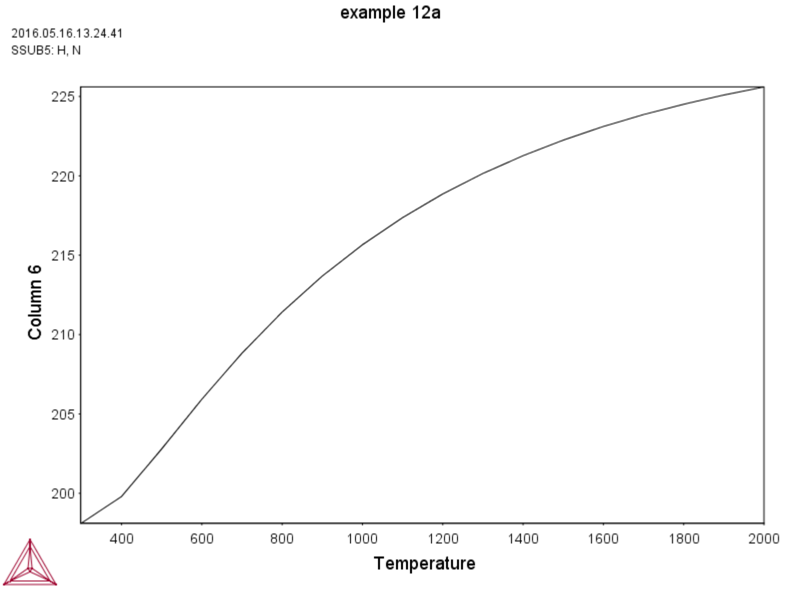
```
About Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex12\tcex12.TCM" set-echo
SYS: @@
SYS: @@ Tabulation
SYS: @@ of thermodynamic data for reactions
SYS: @@
SYS: @@ This example shows a number of independent cases using the
SYS: @@ tabulation module. This module is very rudimentary but still
SYS: @@ provides some facilities. Note that there is no on-line help available!
SYS: @@
SYS: @@ Each case is separated by a line of ============================
SYS: set-log ex12,,
SYS: go tab
   ... the command in full is GOTO_MODULE
TAB: ?
   ... the command in full is HELP
 BACK                     LIST_SUBSTANCES          SWITCH_DATABASE
 ENTER_FUNCTION           MACRO_FILE_OPEN          TABULATE_DERIVATIVES
 ENTER_REACTION           PATCH                    TABULATE_REACTION
 EXIT                     SET_ENERGY_UNIT          TABULATE_SUBSTANCE
 GOTO_MODULE              SET_INTERACTIVE
 HELP                     SET_PLOT_FORMAT
TAB: @@ Tabulate data for a reaction
TAB: tab-rea 3H2+N2=2N1H3;
   ... the command in full is TABULATE_REACTION
 Use one of these databases

 TCFE8    =  Steels/Fe-Alloys  v8.0
 TCFE9    =  Steels/Fe-Alloys  v9.0 SNAPSHOT
 FROST1   =  FROST database v1.0
 TCFE7    =  Steels/Fe-Alloys  v7.0
 TCFE6    =  Steels/Fe-Alloys  v6.2
 TCFE5    =  Steels/Fe-Alloys  v5.0
 TCFE4    =  Steels/Fe-Alloys  v4.1
 TCFE3    =  Steels/Fe-Alloys  v3.1
 TCFE2    =  Steels/Fe-Alloys  v2.1
 TCFE1    =  Steels/Fe-Alloys  v1.0
 FEDAT    =  TCS/TT Steels Database v1.0
 TCNI9    =  Ni-Alloys  v9.0 SNAPSHOT
 TCNI8    =  Ni-Alloys  v8.0
 TCNI7    =  Ni-Alloys  v7.1
 TCNI6    =  Ni-Alloys  v6.0
 TCNI5    =  Ni-Alloys  v5.1
 TCNI4    =  Ni-Alloys  v4.0
 TCNI1    =  Ni-Alloys  v1.3
 TCAL4    =  Al-Alloys  v4.0
 TCAL3    =  Al-Alloys  v3.0
 TCAL2    =  Al-Alloys  v2.0
 TCAL1    =  Al-Alloys  v1.2
 TCMG5    =  Mg-Alloys  v5.0 SNAPSHOT
 TCMG4    =  Mg-Alloys  v4.0
 TCMG3    =  Mg-Alloys  v3.0
 TCMG2    =  Mg-Alloys  v2.0
 TCMG1    =  Mg-Alloys  v1.1
 TCTI1    =  Ti-Alloys  v1.0 SNAPSHOT
 TCCU1    =  Copper  v1.0 SNAPSHOT
 TCCC1    =  Cemented carbide  v1.0
 TCHEA1   =  High Entropy Alloy  v1.0
 SSOL5    =  SGTE Alloy Solutions Database v5.0
 SSOL4    =  SGTE Alloy Solutions Database v4.9f
 SSOL2    =  SGTE Alloy Solutions Database v2.1
 SSUB5    =  SGTE Substances Database v5.1
 SSUB4    =  SGTE Substances Database v4.1
 SSUB3    =  SGTE Substances Database v3.3
 SSUB2    =  SGTE Substances Database v2.2
 SNOB3    =  SGTE Nobel Metal Alloys Database v3.1
 SNOB2    =  SGTE Nobel Metal Alloys Database v2.1
 SNOB1    =  SGTE Nobel Metal Alloys Database v1.2
 STBC2    =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1    =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1    =  SGTE Molten Salts Database v1.2
 SNUX6    =  SGTE In-Vessel Nuclear Oxide TDB v6.2
 SEMC2    =  TC Semi-Conductors  v2.1
 SLAG4    =  Fe-containing Slag  v4.0 snapshot
 SLAG3    =  Fe-containing Slag  v3.2
 SLAG2    =  Fe-containing Slag  v2.2
 SLAG1    =  Fe-containing Slag  v1.2
 TCOX7    =  Metal Oxide Solutions  v7.0 SNAPSHOT
 TCOX6    =  Metal Oxide Solutions  v6.1
 TCOX5    =  Metal Oxide Solutions  v5.1
 TCOX4    =  Metal Oxide Solutions  v4.1
 ION3     =  Ionic Solutions  v3.0
 ION2     =  Ionic Solutions  v2.6
 ION1     =  Ionic Solutions  v1.5
 NOX2     =  NPL Oxide Solutions Database v2.1
 TCSLD3   =  Solder Alloys  v3.1
 TCSLD2   =  Solder Alloys  v2.0
 TCSLD1   =  Solder Alloys  v1.0
 TCSI1    =  Ultrapure Silicon  v1.1
 TCMP2    =  Materials Processing  v2.5
 TCES1    =  Combustion/Sintering  v1.1
 TCSC1    =  Super Conductor  v1.0
 TCFC1    =  SOFC Database v1.0
 TCNF2    =  Nuclear Fuels  v2.1b
 NUMT2    =  Nuclear Materials  v2.1
 NUOX4    =  Nuclear Oxides  v4.2
 NUTO1    =  U-Zr-Si Ternary Oxides TDB v1.1
 NUTA1    =  Ag-Cd-In Ternary Alloys TDB v1.1
 NUCL10   =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH11   =  ThermoData MEPHISTA Nuclear Fuels TDB v11
 TCAQ2    =  Aqueous Solution  v2.5
 AQS2     =  TGG Aqueous Solution Database v2.5
 GCE2     =  TGG Geochemical/Environmental TDB v2.3
 PURE5    =  SGTE Unary (Pure Elements) TDB v5.1
```

```
 ALDEMO  =  Aluminum Demo Database
 FEDEMO  =  Iron Demo Database
 NIDEMO  =  Nickel Demo Database
 SLDEMO  =  Solder Demo Database
 OXDEMO  =  Oxide Demo Database
 SUBDEMO =  Substance Demo Database
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 MOB2    =  Alloys Mobility  v2.4
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0 SNAPSHOT
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database
 MFEDEMO =  Fe-Alloys Mobility demo database
 MNIDEMO =  Ni-Alloys Mobility demo database
 USER    =  User defined Database

DATABASE NAME /TCFE8/: SSUB5
 THERMODYNAMIC DATABASE module
 Current database: SGTE Substances Database v5.1

 VA  DEFINED
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 H2                       N2                       H3N1
   DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      H2<G> H2<G>
      HYDROGEN<G>
      STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   H3N1<G> T.C.R.A.S. Class: 2
      H3N1<G> NH3<G>
      AMMONIA <GAS>
   N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      N2<G> N2<G>
      NITROGEN <DIATOMIC GAS>
      PUBLISHED BY JANAF AT 09/65
 -OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /SCREEN/:

               O U T P U T   F R O M   T H E R M O - C A L C
               2016. 5.16                            13.24.37


 Reaction:  3H2<G>+N2<G>=2H3N1<G>
 H2<GAS>
 N2<GAS>
 H3N1<GAS>

 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04
  800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02   7.72568E+04
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05
 1100.00  -7.77802E+00  -1.11169E+05  -2.34908E+02   1.47229E+05
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05
TAB:Hit RETURN to continue
TAB: @@ Add a final column with a function. In this function
TAB: @@ you may use G, S, H, V, CP, T and R with their obvious
TAB: @@ meaning. You may also use H298 and ALPHA (thermal expansivity)
TAB: @@ and KAPPA (isothermal compressibility). In most databases
TAB: @@ there are no pressure dependence and thus V, ALPHA and KAPPA
TAB: @@ will not be correct.
TAB: e-fun
   ... the command in full is ENTER_FUNCTION
Name: fef
Function: (g-h298)/t
&
TAB: t-r
   ... the command in full is TABULATE_REACTION
```

```
Same reaction? /Y/: y
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /SCREEN/:

               O U T P U T   F R O M   T H E R M O - C A L C
               2016. 5.16                          13.24.37


 Column 6: fef       (G-H298 )/T
 Reaction:  3H2<G>+N2<G>=2H3N1<G>
 H2<GAS>
 N2<GAS>
 H3N1<GAS>

 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04   1.98115E+02
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04   1.98116E+02
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04   1.99799E+02
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03   2.02800E+02
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04   2.05930E+02
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04   2.08834E+02
  800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02   7.72568E+04   2.11421E+02
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05   2.13687E+02
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05   2.15659E+02
 1100.00  -7.77802E+00  -1.11169E+05  -2.34908E+02   1.47229E+05   2.17372E+02
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05   2.18858E+02
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05   2.20149E+02
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05   2.21272E+02
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05   2.22251E+02
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05   2.23107E+02
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05   2.23857E+02
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05   2.24515E+02
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05   2.25093E+02
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05   2.25602E+02
TAB:Hit RETURN to continue
TAB: t-r
   ... the command in full is TABULATE_REACTION
Same reaction? /Y/: y
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /SCREEN/: tcex12a
Grapical output? /Y/: y
Plot column? /2/: 6

               O U T P U T   F R O M   T H E R M O - C A L C
               2016. 5.16                          13.24.37


 Column 6: fef       (G-H298 )/T
 Reaction:  3H2<G>+N2<G>=2H3N1<G>
 H2<GAS>
 N2<GAS>
 H3N1<GAS>

 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04   1.98115E+02
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04   1.98116E+02
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04   1.99799E+02
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03   2.02800E+02
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04   2.05930E+02
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04   2.08834E+02
  800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02   7.72568E+04   2.11421E+02
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05   2.13687E+02
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05   2.15659E+02
 1100.00  -7.77802E+00  -1.11169E+05  -2.34908E+02   1.47229E+05   2.17372E+02
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05   2.18858E+02
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05   2.20149E+02
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05   2.21272E+02
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05   2.22251E+02
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05   2.23107E+02
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05   2.23857E+02
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05   2.24515E+02
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05   2.25093E+02
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05   2.25602E+02


  POSTPROCESSOR VERSION 3.2

   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is SET_SCALING_STATUS
   ... the command in full is PLOT_DIAGRAM
```



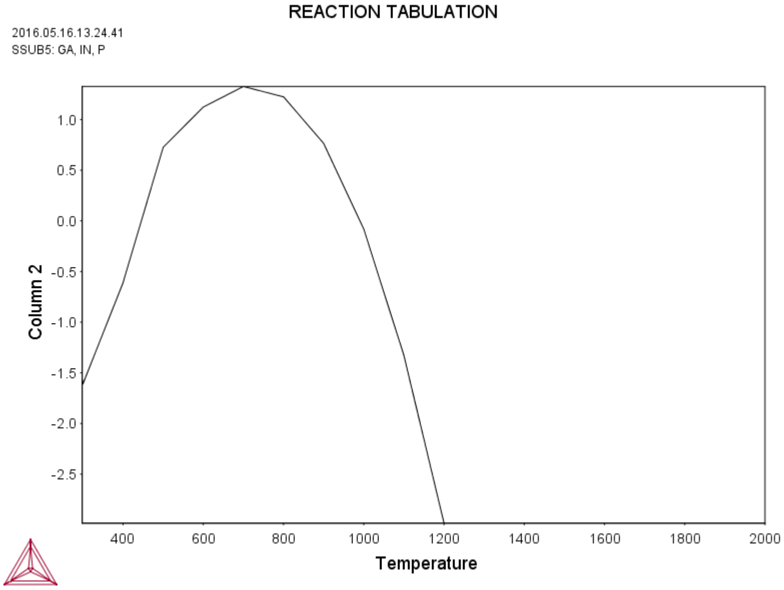
```
POST:
POST: set-title example 12a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



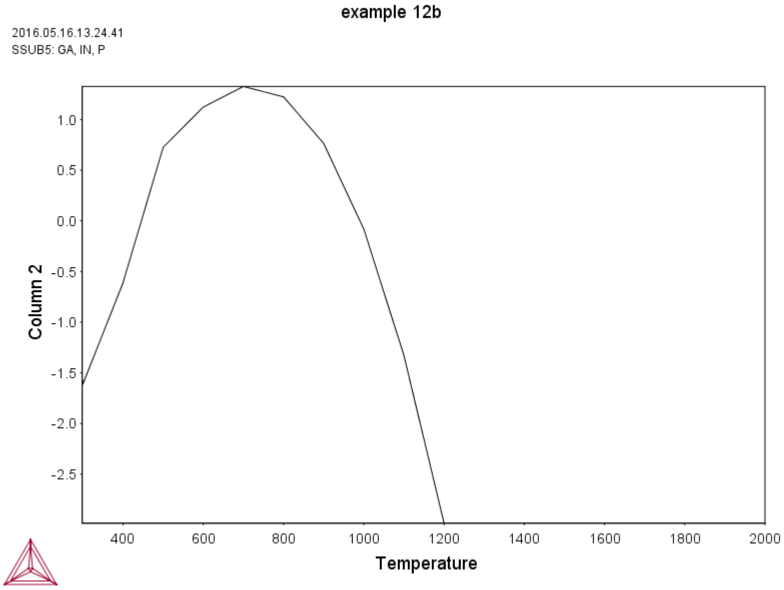
```
POST:
POST:Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ In the Gibbs-Enery-System we can list the data we use
TAB: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: l-d
   ... the command in full is LIST_DATA
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?: ?

 OPTIONS?

  Choose one or several of the following options for output:
   * N  the output is written as a ''user'' database format.
   * P  the output is written as a MACRO file for future input.
          This is useful for creating setup files for assessments.
   * S  the symbols are suppressed.
   * R  the references for the parameters are listed
          (only for some databases in which references are available)
   * L  the output is written suitable for a LaTeX preprocessor.


OPTIONS?: rs

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE: SSUB5

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 H    1/2_MOLE_H2(GAS)          1.0079E+00  4.2340E+03  6.5285E+01
  2 N    1/2_MOLE_N2(GAS)          1.4007E+01  4.3350E+03  9.5751E+01


 SPECIES                                    STOICHIOMETRY
   1 H                                      H
   2 H2                                     H2
```

```
   3 H3N1                                    H3N1
   4 N                                       N
   5 N2                                      N2
   6 VA                                      VA



 GAS
    CONSTITUENTS: H2,H3N1,N2

      G(GAS,H2;0)- 2 H298(1/2_MOLE_H2(GAS),H;0) = +F11227T+R*T*LN(1E-05*P)
           REFERENCE: 9480
      G(GAS,H3N1;0)- 3 H298(1/2_MOLE_H2(GAS),H;0)-H298(1/2_MOLE_N2(GAS),N;0)
           = +F11369T+R*T*LN(1E-05*P)
           REFERENCE: 9537
      G(GAS,N2;0)- 2 H298(1/2_MOLE_N2(GAS),N;0) = +F13668T+R*T*LN(1E-05*P)
           REFERENCE:11534

 LIST_OF_REFERENCES
 NUMBER  SOURCE
   REF9480   H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
           H2<G> H2<G>
           HYDROGEN<G>
           STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   REF9537   H3N1<G> T.C.R.A.S. Class: 2
           H3N1<G> NH3<G>
           AMMONIA <GAS>
   REF11534  N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
           N2<G> N2<G>
           NITROGEN <DIATOMIC GAS>
           PUBLISHED BY JANAF AT 09/65

GES:Hit RETURN to continue
GES: back
TAB:
TAB: @@ Tabulate another reaction ===============================================
TAB: t-r
   ... the command in full is TABULATE_REACTION
Same reaction? /Y/: n
Reaction: INP+GA=GAP+IN;
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 GA                      IN1P1                   IN
 GA1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   GA1<G> T.C.R.A.S. Class: 1
      GA1<G> Ga<G>
      GALLIUM <GAS>
   GA1P1<G> S.G.T.E.
      GA1P1<G> GaP<G>
      GALLIUM PHOSPHIDE <GAS>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
      from T.C.R.A.S.
   IN1<G> THERMODATA
      IN1<G> In<G>
      New Assessment (H_form and S only)
   IN1P1<G> CHATILLON(1994 March)
      IN1P1<G> InP<G>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   GA1P1 S.G.T.E.
      GA1P1 GaP
      GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
   GA1 S.G.T.E. **
      GA1 Ga
      GALLIUM
      Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
      20080211 BC Tref 200 -> 298.15
   IN1P1 I. BARIN 3rd. Edition
      IN1P1 InP
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
   IN1 S.G.T.E. **
      IN1 In
      INDIUM
      Data from SGTE Unary DB
 -OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /tcex12a/: tcex12b
Grapical output? /Y/: Y
Plot column? /2/: 2

               O U T P U T   F R O M   T H E R M O - C A L C
               2016. 5.16                           13.24.41


 Column 6: fef       (G-H298 )/T
 Reaction:  GA+IN1P1=IN+GA1P1
 GA stable as GA_S
 IN1P1 stable as IN1P1_S
 IN stable as IN_S
 GA1P1 stable as GA1P1_S

 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  298.15  -1.56785E+00  -4.01610E+04   4.46600E+00  -4.14925E+04  -4.46600E+00
  300.00  -1.60915E+00  -4.01639E+04   4.45617E+00  -4.15008E+04  -4.46597E+00
  302.   ---- GA becomes GA_L ,delta-H =   5589.80
  400.00  -6.09329E-01  -4.59820E+04  -1.46756E+01  -4.01118E+04   1.23002E-01
```

```
  430.   ---- IN becomes IN_L ,delta-H =   3283.00
  500.00   7.26020E-01  -4.26605E+04  -6.95385E+00  -3.91835E+04   1.95492E+00
  600.00   1.12393E+00  -4.25671E+04  -6.78469E+00  -3.84963E+04   2.77457E+00
  700.00   1.32655E+00  -4.24423E+04  -6.59282E+00  -3.78274E+04   3.33376E+00
  800.00   1.22407E+00  -4.23120E+04  -6.41862E+00  -3.71771E+04   3.72988E+00
  900.00   7.64029E-01  -4.22095E+04  -6.29733E+00  -3.65419E+04   4.02125E+00
 1000.00  -8.12013E-02  -4.21720E+04  -6.25712E+00  -3.59149E+04   4.24608E+00
 1100.00  -1.32730E+00  -4.22391E+04  -6.32007E+00  -3.52870E+04   4.43091E+00
 1200.00  -2.98369E+00  -4.24512E+04  -6.50358E+00  -3.46469E+04   4.59509E+00
 Temperature range exceeded for IN1P1

   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is SET_SCALING_STATUS
   ... the command in full is PLOT_DIAGRAM
```



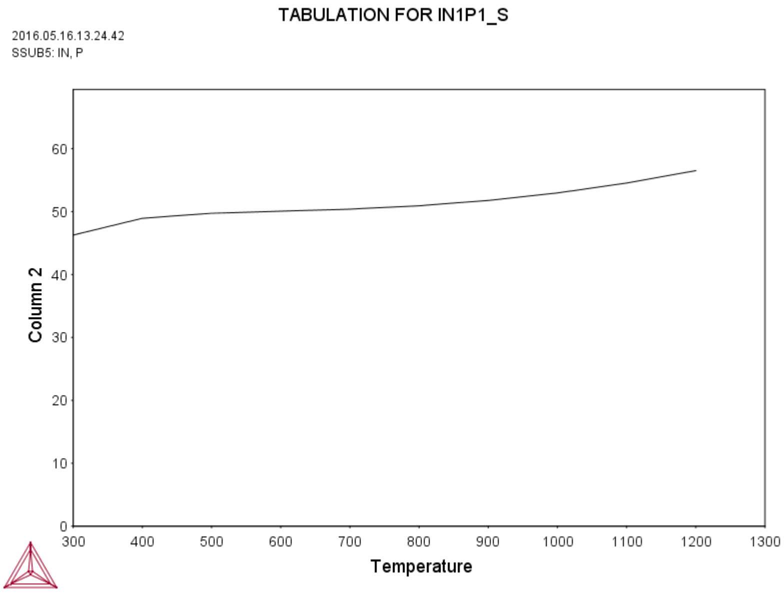
```
POST:
POST: set-title example 12b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



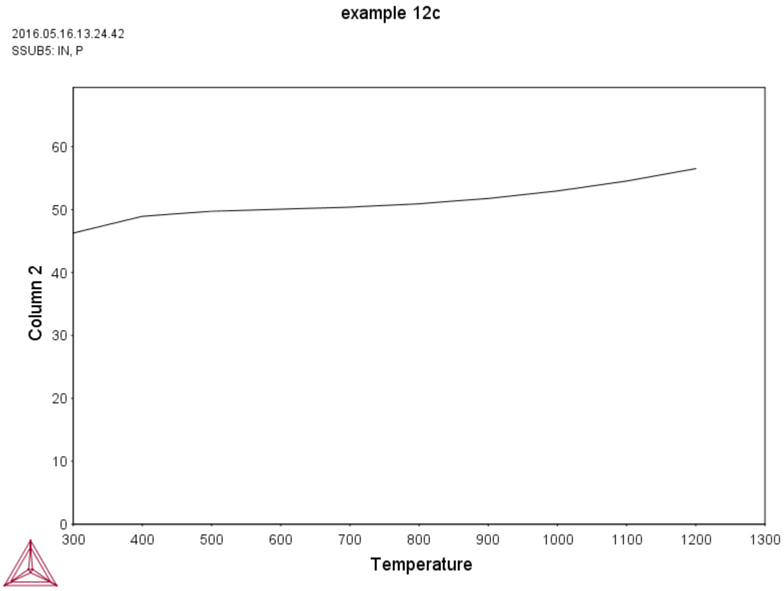
```
POST:
POST:Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ By default a species in a gas is not included in
TAB: @@ a tabulation, you must specify <GAS> if you want that
TAB: t-r n
   ... the command in full is TABULATE_REACTION
Reaction: INP<gas>+GA=GAP+IN;
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 GA                      IN1P1                   IN
 GA1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   GA1<G> T.C.R.A.S. Class: 1
      GA1<G> Ga<G>
      GALLIUM <GAS>
   GA1P1<G> S.G.T.E.
      GA1P1<G> GaP<G>
```

```
      GALLIUM PHOSPHIDE <GAS>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
      from T.C.R.A.S.
   IN1<G> THERMODATA
      IN1<G> In<G>
      New Assessment (H_form and S only)
   IN1P1<G> CHATILLON(1994 March)
      IN1P1<G> InP<G>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   GA1P1 S.G.T.E.
      GA1P1 GaP
      GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
   GA1 S.G.T.E. **
      GA1 Ga
      GALLIUM
      Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
      20080211 BC Tref 200 -> 298.15
   IN1P1 I. BARIN 3rd. Edition
      IN1P1 InP
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
   IN1 S.G.T.E. **
      IN1 In
      INDIUM
      Data from SGTE Unary DB
 -OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 1000
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /tcex12b/:
Grapical output? /Y/: N

               O U T P U T  F R O M  T H E R M O - C A L C
               2016. 5.16                           13.24.42


 Column 6: fef       (G-H298 )/T
 Reaction:  GA+IN1P1<G>=IN+GA1P1
 GA stable as GA_L
 IN1P1<GAS>
 IN1P1<GAS>
 IN stable as IN_L
 GA1P1 stable as GA1P1_S

 *******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 *******************************************************************************
 1000.00   1.57503E+01  -4.65760E+05  -1.78780E+02  -2.86980E+05   1.86368E+02
 1100.00   1.60263E+01  -4.64172E+05  -1.77266E+02  -2.69179E+05   1.85608E+02
 1200.00   1.63030E+01  -4.62555E+05  -1.75860E+02  -2.51523E+05   1.84854E+02
 1300.00   1.65828E+01  -4.60911E+05  -1.74544E+02  -2.34004E+05   1.84111E+02
 1400.00   1.68674E+01  -4.59238E+05  -1.73305E+02  -2.16612E+05   1.83383E+02
 1500.00   1.71578E+01  -4.57537E+05  -1.72131E+02  -1.99341E+05   1.82672E+02
 1600.00   1.74548E+01  -4.55807E+05  -1.71014E+02  -1.82184E+05   1.81978E+02
 1700.00   1.77582E+01  -4.54046E+05  -1.69947E+02  -1.65136E+05   1.81301E+02
 Temperature range exceeded for GA1P1
TAB:Hit RETURN to continue
TAB: @@ ======================================================================
TAB: @@ You can list substances in the database
TAB: li-sub
   ... the command in full is LIST_SUBSTANCES
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 AG  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   AG1<G> THERMODATA
      AG1<G> Ag<G>
      SILVER <GAS>
      Modified Thermodata new assessment
   AG1 HULTGREN SELECTED VAL. SGTE **
      AG1 Ag
      SILVER
      CODATA KEY VALUE.MPT=1234.93K.
      --U.D. 30/10/85 .
 -OK-
With elements /*/: IN P
Exclusivly with those elements? /Y/:
IN                      P                       IN2
IN1P1                   P2                      P3
P4
TAB: @@ or all substances with Fe
TAB: li-sub
   ... the command in full is LIST_SUBSTANCES
With elements /*/: FE
Exclusivly with those elements? /Y/: N
FE                      AL2FE1O4                AS1FE1O4
AS2FE3O8                B1FE1                   B1FE2
BA1FE1ND1O4             BA1FE2ND2O7             BR1FE1
BR2FE1                  BR3FE1                  BR4FE2
BR6FE2                  C1FE1O3                 C1FE3
C5FE1O5                 CA1FE2O4                CA2FE2O5
CD1FE2O4                CL1FE1                  CL1FE1O1
CL2FE1                  CL3FE1                  CL4FE2
CL6FE2                  CO1FE2O4                CR2FE1O4
CU1FE1O2                CU1FE1S2                CU1FE2O4
CU2FE2O4                CU5FE1S4                F1FE1
F2FE1                   F3FE1                   F4FE2
F6FE2                   FE1/+1                  FE1/-1
FE2                     FE1H1                   FE1H1O1
FE1H1O2                 FE2H2O4                 FE1H2O2
FE1H3O3                 FE0.947O1               FE1O1
```

```
FE1O2                   FE2O3                   FE3O4
FE0.875S1               FE1S1                   FE1S2
FE1O4S1                 FE2O12S3                FE1SE0.96
FE1.04SE1               FE1SE1                  FE1SE2
FE2N1                   FE4N1                   FE1P1
FE1P2                   FE2P1                   FE3P1
FE1H4O6P1               FE1I1                   FE1I2
FE1I3                   FE2I4                   FE2I6
FE1K1O2                 FE1K2O2                 FE1K4O3
FE1LI1O2                FE1LI5O4                FE1MO1O4
FE1NA1O2                FE1O3SI1                FE1O3TI1
FE1O4V2                 FE1O4W1                 FE1O6V2
FE1SI1                  FE1SI2.33               FE1SI2
FE1TE0.9                FE1TE1                  FE1TE2
FE1TI1                  FE2LI2O4                FE2MG1O4
FE2MN1O4                FE2NB1                  FE2NI1O4
FE2O4SI1                FE2O4TI1                FE2O4ZN1
FE2TA1                  FE2TI1                  FE2U1
FE3LI2O5                FE3MO2                  FE3W2
FE5LI1O8
TAB:
TAB:Hit RETURN to continue
TAB: @@ ======================================================================
TAB: @@ You can tabulate data for a substance or phase also, this is equivalent
TAB: @@ with tabels you may find in JANAF for example
TAB: t-sub IN1P1
   ... the command in full is TABULATE_SUBSTANCE
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 IN1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   IN1P1<G> CHATILLON(1994 March)
      IN1P1<G> InP<G>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   IN1P1 I. BARIN 3rd. Edition
      IN1P1 InP
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
 -OK-
Pressure /100000/: 100000
Low temperature limit /1000/: 300
High temperature limit /2000/: 1300
Step in temperature /100/: 100
Output file /tcex12b/: tcex12c
Grapical output? /Y/: Y
Plot column? /2/: 2

               O U T P U T  F R O M  T H E R M O - C A L C
               2016. 5.16                           13.24.42


 Column 6: fef       (G-H298 )/T

 Phase : IN1P1_S                    Pressure :      100000.00
 Specie: IN1P1

 ******************************************************************************
    T      Cp            H             S             G            fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  300.00   4.62734E+01  -7.44015E+04   6.42060E+01  -9.36633E+04  -6.39209E+01
  400.00   4.89412E+01  -6.96137E+04   7.79614E+01  -1.00798E+05  -6.57782E+01
  500.00   4.97376E+01  -6.46723E+04   8.89845E+01  -1.09165E+05  -6.93552E+01
  600.00   5.00615E+01  -5.96811E+04   9.80837E+01  -1.18531E+05  -7.34072E+01
  700.00   5.03923E+01  -5.46595E+04   1.05824E+02  -1.28736E+05  -7.74989E+01
  800.00   5.09302E+01  -4.95956E+04   1.12585E+02  -1.39664E+05  -8.14708E+01
  900.00   5.17709E+01  -4.44633E+04   1.18629E+02  -1.51229E+05  -8.52694E+01
 1000.00   5.29647E+01  -3.92297E+04   1.24142E+02  -1.63372E+05  -8.88848E+01
 1100.00   5.45403E+01  -3.38577E+04   1.29261E+02  -1.76045E+05  -9.23252E+01
 1200.00   5.65148E+01  -2.83083E+04   1.34088E+02  -1.89214E+05  -9.56061E+01
 Temperature range exceeded
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is PLOT_DIAGRAM
```

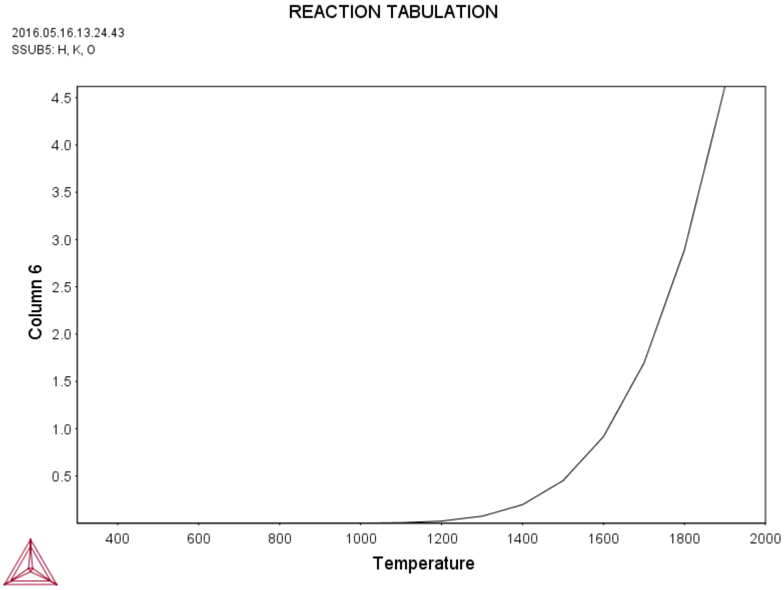


```
POST:Hit RETURN to continue
POST:
POST: set-title example 12c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

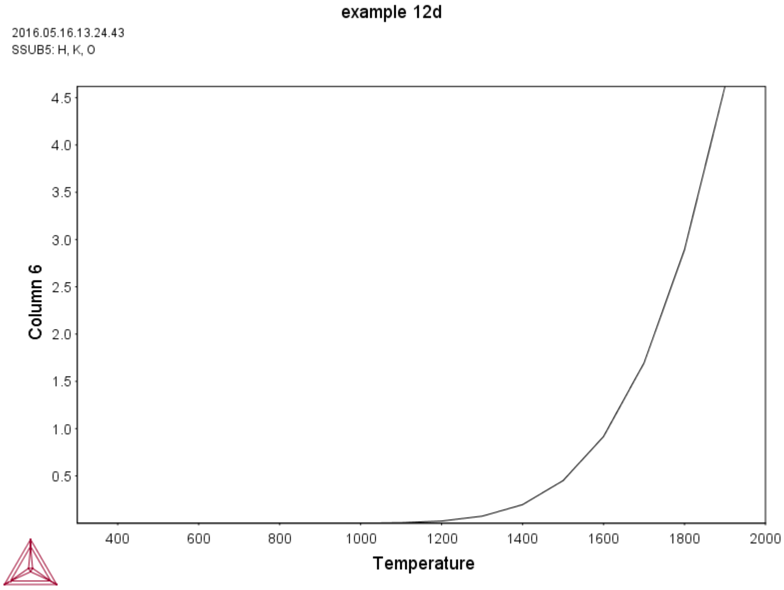


```
POST:
POST:Hit RETURN to continue
POST: back

TAB: @@ ======================================================================
TAB: @@ In order to obtain the partial pressure of a species in
TAB: @@ the gas in its pure condenced state you can enter a reaction
TAB: @@ like this for KOH. The partial pressure is entered as a
TAB: @@ function exp(-G/R/T)
TAB: e-fun
   ... the command in full is ENTER_FUNCTION
Name: pp
Function: exp(-g/r/t);
TAB:
TAB: tab-r n K1O1H1=K1H1O1<g>
   ... the command in full is TABULATE_REACTION
&
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 H1K1O1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   H1K1O1<G> J. Phys. Chem. Ref. Data
      H1K1O1<G> KOH<G>
      Data taken from JPCRD, 26, 4 1031-1110 (1997)
   H1K1O1 J. Phys. Chem. Ref. Data
      H1K1O1 KOH
      Data taken from JPCRD, 26, 4 1031-1110 (1997)
 -OK-
Pressure /100000/: 100000
Low temperature limit /300/: 300
High temperature limit /1300/: 2000
Step in temperature /100/: 100
```

```
Output file /tcex12c/: tcex12d
Grapical output? /Y/: Y
Plot column? /2/: 6

              O U T P U T   F R O M   T H E R M O - C A L C
              2016. 5.16                           13.24.42


 Column 6: pp         EXP(-G/R/T )
 Reaction:  H1K1O1=H1K1O1<G>
 H1K1O1 stable as H1K1O1_S
 H1K1O1<GAS>

 *****************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       pp
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 *****************************************************************************
  300.00  -1.97899E+01   1.92543E+05   1.56915E+02   1.45469E+05   4.70147E-26
  400.00  -2.31294E+01   1.90409E+05   1.50797E+02   1.30090E+05   1.02900E-17
  500.00  -2.73216E+01   1.87890E+05   1.45195E+02   1.15293E+05   9.03075E-13
  517.   ---- H1K1O1 becomes H1K1O1_S2 ,delta-H =   5600.00
  600.00  -2.71797E+01   1.79542E+05   1.29351E+02   1.01932E+05   1.33747E-09
  680.   ---- H1K1O1 becomes H1K1O1_L ,delta-H =   7900.00
  700.00  -3.36564E+01   1.68804E+05   1.13354E+02   8.94566E+04   2.11269E-07
  800.00  -3.31914E+01   1.65462E+05   1.08890E+02   7.83499E+04   7.66317E-06
  900.00  -3.27453E+01   1.62165E+05   1.05007E+02   6.76592E+04   1.18375E-04
 1000.00  -3.22973E+01   1.58913E+05   1.01580E+02   5.73333E+04   1.01226E-03
 1100.00  -3.18358E+01   1.55706E+05   9.85231E+01   4.73310E+04   5.65583E-03
 1200.00  -3.13536E+01   1.52547E+05   9.57735E+01   3.76185E+04   2.30437E-02
 1300.00  -3.08482E+01   1.49436E+05   9.32837E+01   2.81676E+04   7.38312E-02
 1400.00  -3.03294E+01   1.46378E+05   9.10171E+01   1.89543E+04   1.96257E-01
 1500.00  -2.98854E+01   1.43368E+05   8.89402E+01   9.95788E+03   4.50033E-01
 1600.00  -2.94990E+01   1.40399E+05   8.70240E+01   1.16091E+03   9.16434E-01
 1700.00  -2.91580E+01   1.37467E+05   8.52461E+01  -7.45152E+03   1.69415E+00
 1800.00  -2.88535E+01   1.34567E+05   8.35882E+01  -1.58923E+04   2.89182E+00
 1900.00  -2.85787E+01   1.31695E+05   8.20357E+01  -2.41727E+04   4.61888E+00
 Temperature range exceeded for H1K1O1

   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is SET_SCALING_STATUS
   ... the command in full is PLOT_DIAGRAM
```

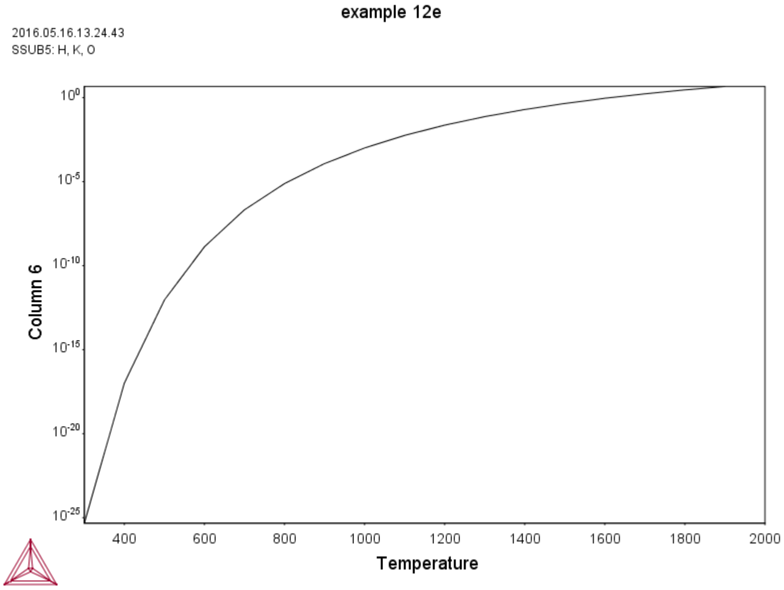


```
POST:
POST: set-title example 12d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
```

```
POST: s-a-ty y
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 12e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



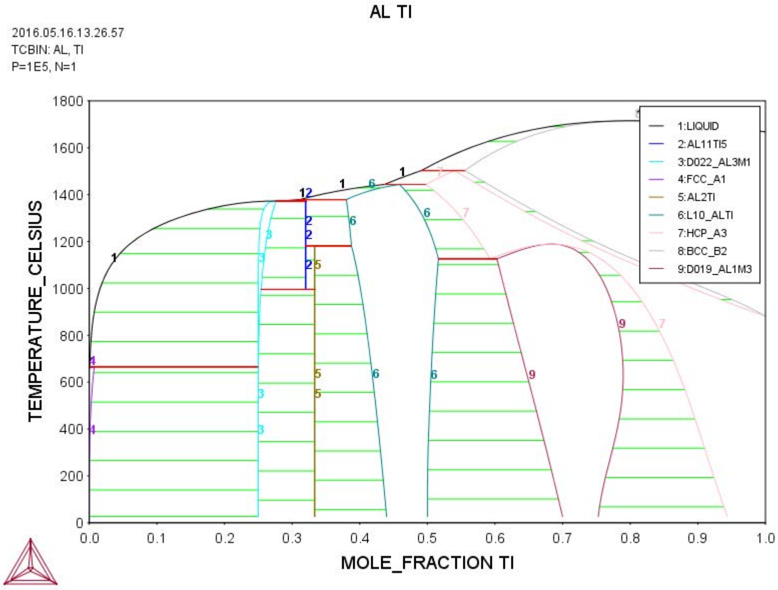
```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex13

```
About
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex13\tcex13.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation
SYS: @@ of phase diagram and G curve
SYS: @@ using the BINARY module
SYS: @@
SYS: @@ Binary Al-Ti phase diagram and G curve
SYS: @@
SYS: set-log ex13,,,
SYS: GO BIN
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC Binary Solutions  v1.1

 VA                      /-   DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: ?
 The following assessed systems
  AG-AL AG-AU AG-BI AG-CU AG-GE AG-IN AG-IR AG-MG AG-OS AG-PB AG-PD AG-PT
  AG-RH AG-RU AG-SB AG-SI AG-SN AG-TI AG-TL AG-ZN AG-ZR AL-AS AL-AU  AL-B
  AL-BI  AL-C AL-CA AL-CE AL-CO AL-CR AL-CU AL-FE AL-GA AL-GE AL-IN AL-LI
  AL-MG AL-MN AL-MO  AL-N AL-NB AL-ND AL-NI  AL-O  AL-P AL-PB AL-SB AL-SI
  AL-SN AL-TA AL-TI  AL-V  AL-W  AL-Y AL-ZN AL-ZR AS-AU AS-CU AS-FE AS-GA
  AS-GE AS-IN  AS-P AS-SB AU-BI  AU-C AU-CR AU-CU AU-GE AU-IN AU-PB AU-PD
  AU-RH AU-RU AU-SB AU-SI AU-TE AU-TL   B-C  B-CO  B-CR  B-FE  B-HF  B-MG
  B-MO   B-N  B-ND  B-NI  B-SC  B-SI  B-TI   B-V   B-W BA-CU BA-EU BA-SR
  BA-Y BI-CU BI-GA BI-GE BI-HG BI-IN  BI-K BI-MG  BI-O BI-PB BI-SB BI-SI
  BI-SN BI-TL BI-ZN  C-CO  C-CR  C-CU  C-FE  C-HF  C-MN  C-MO  C-NB  C-NI
  C-PB  C-SI  C-TA  C-TI   C-V   C-W   C-Y  C-ZR CA-CU CA-MG CA-PB CA-SI
  CA-ZN CD-GA CD-GE CD-HG CD-IN CD-PB CD-SB CD-SN CD-TE CD-ZN CE-MG CO-CR
  CO-CU CO-DY CO-FE CO-IN CO-MN CO-MO  CO-N CO-NB CO-NI CO-PD CO-PT CO-SI
  CO-TA CO-TI  CO-V  CO-W CR-CU CR-FE CR-MG CR-MN CR-MO CR-N CR-NB CR-NI
  CR-P CR-PD CR-PT CR-SI CR-SN CR-TA CR-TI  CR-V  CR-W CR-ZN CR-ZR  CS-K
  CS-NA CS-RB CU-FE CU-GE CU-IN CU-LI CU-MG CU-MN CU-N CU-NB CU-NI  CU-O
  CU-P CU-PB  CU-S CU-SB CU-SI CU-SN CU-SR CU-TI CU-TL  CU-V  CU-Y CU-ZN
  CU-ZR DY-ER DY-HO ER-HO ER-TB FE-MG FE-MN FE-MO  FE-N FE-NB FE-ND FE-NI
  FE-O  FE-P FE-PB FE-PD FE-PR FE-PT  FE-S FE-SI FE-SN FE-TI  FE-V  FE-W
  FE-ZN FE-ZR GA-GE GA-HG GA-IN GA-P GA-PB GA-SB GA-SN GA-TE GA-ZN GE-IN
  GE-PB GE-SB GE-SI GE-SN GE-TE GE-TL GE-ZN  H-NB  H-ZR HF-TA HF-SI HF-TI
  HG-PB HO-TB  IN-P IN-PB IN-SB IN-SI IN-SN IN-ZN IR-PD  K-RB LA-NI LI-MG
  LI-ZR MG-MN MG-NI  MG-O MG-SC MG-SI  MG-Y MG-ZN MG-ZR MN-MO  MN-N  MN-O
  MN-PB MN-SI MN-TI  MN-V  MN-Y MN-ZR  MO-N MO-NB MO-NI MO-SI MO-TA MO-TI
  MO-W  N-NB  N-NI  N-TA  N-TI   N-V   N-W NA-RB NB-NI  NB-O NB-TI  NB-V
  NB-W NB-ZR ND-PR ND-SB  NI-P NI-PD NI-SI NI-TA NI-TI  NI-V  NI-W  NI-Y
  NI-ZR  O-PB  O-SN  O-SR  O-TI   O-Y  O-ZR  P-SB  P-SI PB-PD PB-SB PB-SI
  PB-SN PB-TL PB-ZN PD-RU PD-SN PR-SB PT-RH PT-RU RE-TA RE-W SB-SI SB-SN
  SB-ZN SE-SN SE-TE SE-TL SI-SN SI-TA SI-TE SI-TI  SI-U  SI-V  SI-W  SI-Y
  SI-ZN SI-ZR SN-TI SN-ZN SN-ZR TA-TI  TA-V  TA-W TA-ZR TE-ZN  TI-V  TI-W
  TI-ZR  U-ZR  V-ZR  Y-ZR

First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:
   ... the command in full is REJECT
 VA                      /-   DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 AL                      TI  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  CBCC_A12                CUB_A13
 B11_CUTI                B32_ALLI                C14_LAVES
 C15_LAVES               C16_AL2CU               C36_LAVES
 D019_AL1M3              D019_SNTI3              D022_AL3M1
 D1A_CU4TI               D513_AL3NI2             D88_SI3TI5
 L10_ALTI                AL11TI5                 AL2TI
 AL5FE4                  ALCE_AMORPHOUS          MTI2
   REJECTED
 LIQUID:L  RESTORED
 AL11TI5  RESTORED
 AL2TI  RESTORED
 D022_AL3M1  RESTORED
 D019_AL1M3  RESTORED
 L10_ALTI  RESTORED
 A2_BCC  RESTORED
 BCC_B2  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'N Saunders, COST 507 (1998) ISBN 92-828-3902-8 p 89-94; Al-Ti'
  'N. Dupin, 1999, lattice stability for G(BCC_A2,VA:VA)'
  'N. Dupin, I. Ansara, Z. metallkd., Vol 90 (1999) p 76-85; Al-Ni'
  'A V Davydov et al, Metall Mater Trans 32A (2001)9 p 2175-2186; Co-Ti'
```

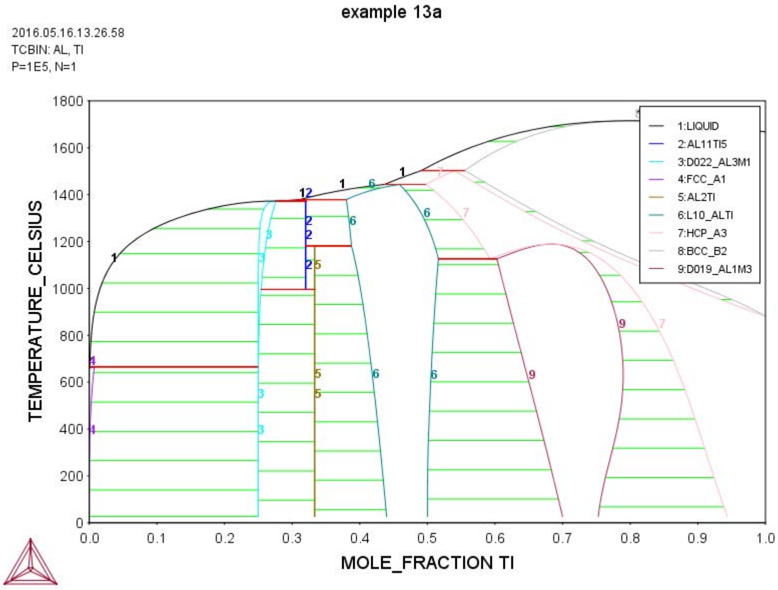
```
 'B Sundman, fix to avoid BCC with just Va (2001)'
 'B Sundman, Set to zero due to the phase partitioning model '
-OK-
  ... the command in full is SET_AXIS_VARIABLE
The condition X(TI)=.1234  created
  ... the command in full is SET_AXIS_VARIABLE
The condition T=1319.08  created
  ... the command in full is SET_REFERENCE_STATE
  ... the command in full is SET_REFERENCE_STATE
  ... the command in full is SAVE_WORKSPACES
  ... the command in full is SET_CONDITION
  ... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
  ... the command in full is COMPUTE_EQUILIBRIUM
  ... the command in full is COMPUTE_EQUILIBRIUM
Start points provided by database
  ... the command in full is SAVE_WORKSPACES
Version S mapping is selected

Organizing start points

Generating start point   1
Generating start point   2

Phase region boundary   1 at:   4.169E-01  1.704E+03
    LIQUID
 ** L10_ALTI
Calculated.                      7  equilibria

Phase region boundary   2 at:   3.454E-01  1.652E+03
    LIQUID
 ** AL11TI5
 ** L10_ALTI

Phase region boundary   3 at:   3.153E-01  1.652E+03
    LIQUID
 ** AL11TI5
Calculated.                      3  equilibria

Phase region boundary   4 at:   3.016E-01  1.646E+03
    LIQUID
 ** AL11TI5
 ** D022_AL3M1

Phase region boundary   5 at:   2.797E-01  1.646E+03
    LIQUID
 ** D022_AL3M1
Calculated.                     36  equilibria

Phase region boundary   6 at:   1.254E-01  9.380E+02
    LIQUID
 ** D022_AL3M1
 ** FCC_A1

Phase region boundary   7 at:   4.025E-03  9.380E+02
    LIQUID
 ** FCC_A1
Calculated                     12  equilibria

Phase region boundary   8 at:   1.287E-01  9.380E+02
    D022_AL3M1
 ** FCC_A1
Calculated..                     27  equilibria
Terminating at axis limit.

Phase region boundary   9 at:   2.981E-01  1.646E+03
    AL11TI5
 ** D022_AL3M1
Calculated.                     17  equilibria

Phase region boundary  10 at:   2.871E-01  1.269E+03
    AL11TI5
 ** AL2TI
 ** D022_AL3M1

Phase region boundary  11 at:   3.267E-01  1.269E+03
    AL11TI5
 ** AL2TI
Calculated.                      9  equilibria

Phase region boundary  12 at:   3.267E-01  1.454E+03
    AL11TI5
 ** AL2TI
 ** L10_ALTI

Phase region boundary  13 at:   3.539E-01  1.454E+03
    AL11TI5
 ** L10_ALTI
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   3.605E-01  1.454E+03
    AL2TI
 ** L10_ALTI
Calculated..                     48  equilibria
Terminating at axis limit.

Phase region boundary  15 at:   2.937E-01  1.269E+03
 ** AL2TI
    D022_AL3M1
Calculated..                     40  equilibria
Terminating at axis limit.

Phase region boundary  16 at:   3.454E-01  1.652E+03
    LIQUID
 ** L10_ALTI
Calculated.                      9  equilibria

Phase region boundary  17 at:   4.476E-01  1.717E+03
    LIQUID
 ** HCP_A3
 ** L10_ALTI

Phase region boundary  18 at:   4.672E-01  1.717E+03
    LIQUID
```

```
  ** HCP_A3
 Calculated.                       4  equilibria

 Phase region boundary  19 at:   5.157E-01  1.776E+03
     LIQUID
  ** BCC_B2
  ** HCP_A3

 Phase region boundary  20 at:   5.233E-01  1.776E+03
     LIQUID
  ** BCC_B2
 Calculated                      43  equilibria

 Phase region boundary  21 at:   5.477E-01  1.776E+03
  ** BCC_B2
     HCP_A3
 Calculated                      41  equilibria

 Phase region boundary  22 at:   4.784E-01  1.717E+03
  ** HCP_A3
     L10_ALTI
 Calculated.                      14  equilibria

 Phase region boundary  23 at:   5.545E-01  1.399E+03
  ** D019_AL1M3
  ** HCP_A3
     L10_ALTI

 Phase region boundary  24 at:   5.596E-01  1.399E+03
  ** D019_AL1M3
     L10_ALTI
 Calculated..                      45  equilibria
 Terminating at axis limit.

 Phase region boundary  25 at:   5.977E-01  1.399E+03
  ** D019_AL1M3
     HCP_A3
 Calculated..                      63  equilibria
 Terminating at axis limit.

 Phase region boundary  26 at:   4.169E-01  1.704E+03
     LIQUID
  ** L10_ALTI
 Calculated.                       4  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex13\BINA
 RY.POLY3
 CPU time for mapping                       2  seconds

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes


  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

   ... the command in full is SET_TIELINE_STATUS
   ... the command in full is SET_LABEL_CURVE_OPTION
   ... the command in full is PLOT_DIAGRAM
```

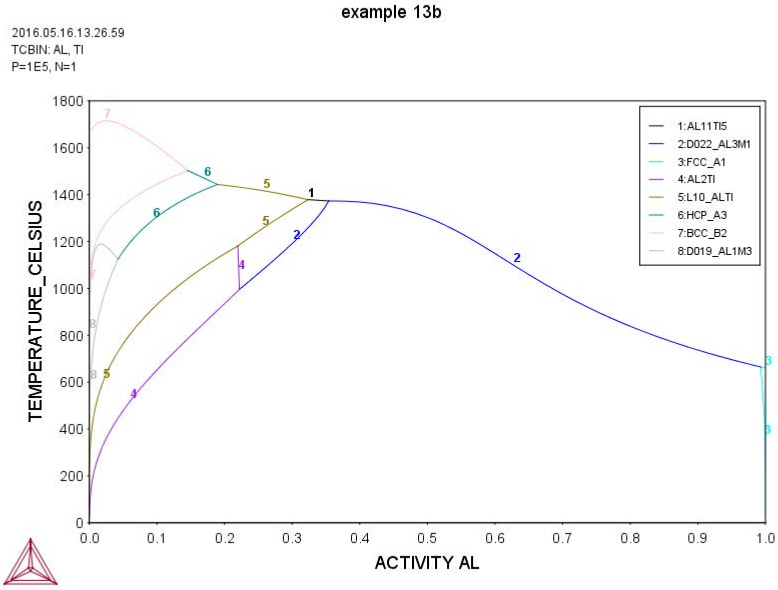


```
POST: @@ Set some phase labels
POST: ADD
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .7 1400
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated          5763 grid points in              0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution        1 s, total time     1  s
 Stable phases are: BCC_B2
Text size: /.36/: ADD

 *** ERROR  1034 IN GETREL
 *** NO DIGIT
POST: .51 400
  No such command, use HELP
POST:
```

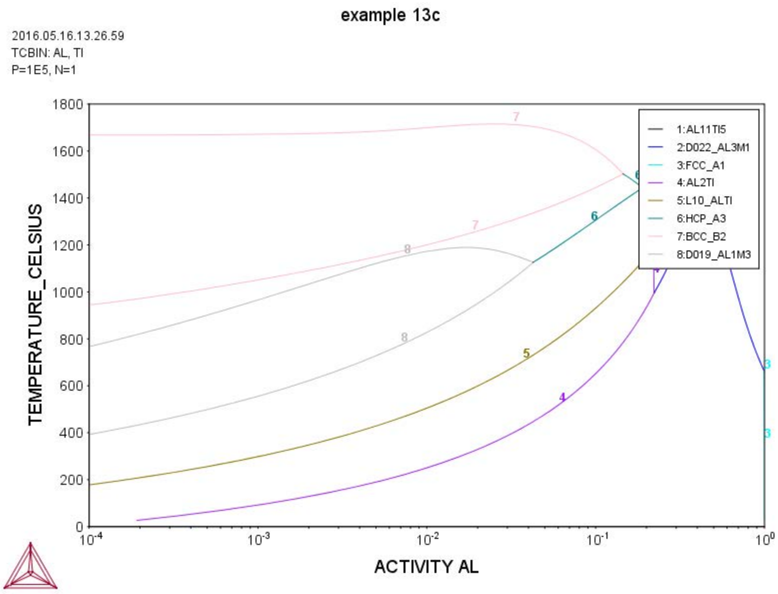
```
POST: set-title example 13a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



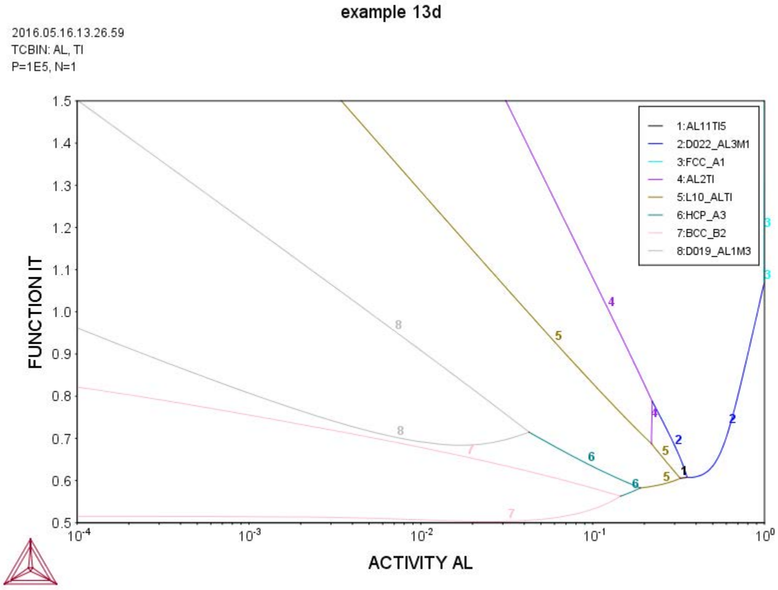
```
POST:
POST:Hit RETURN to continue
POST: @@ We may plot the activites as well
POST: S-D-A
   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : X
VARIABLE : AC
FOR COMPONENT : AL
POST: s-l e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: S-A-TY X
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: LOG
POST: S-S X N 1E-4 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 13c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

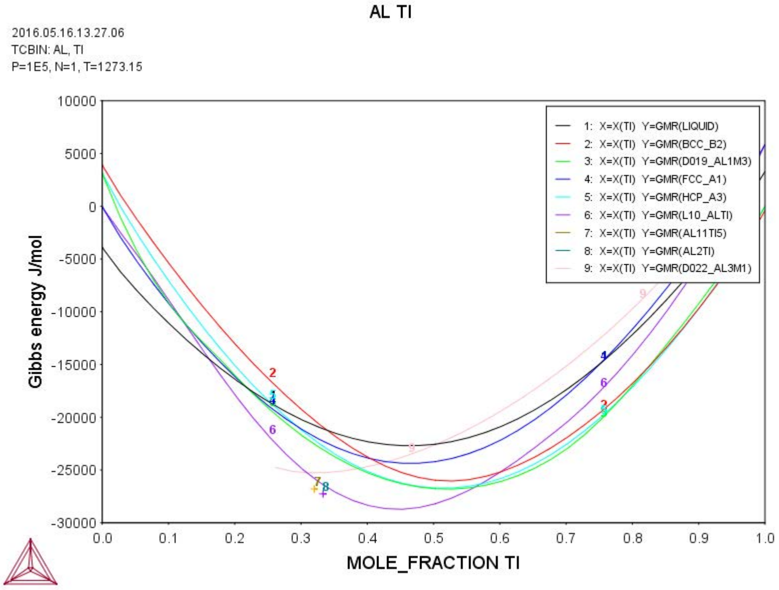


```
POST:
POST:Hit RETURN to continue
POST: @@ Now use inverse of T as y axis
POST: ent fun it=1000/T;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y it
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n .5 1.5
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 13d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

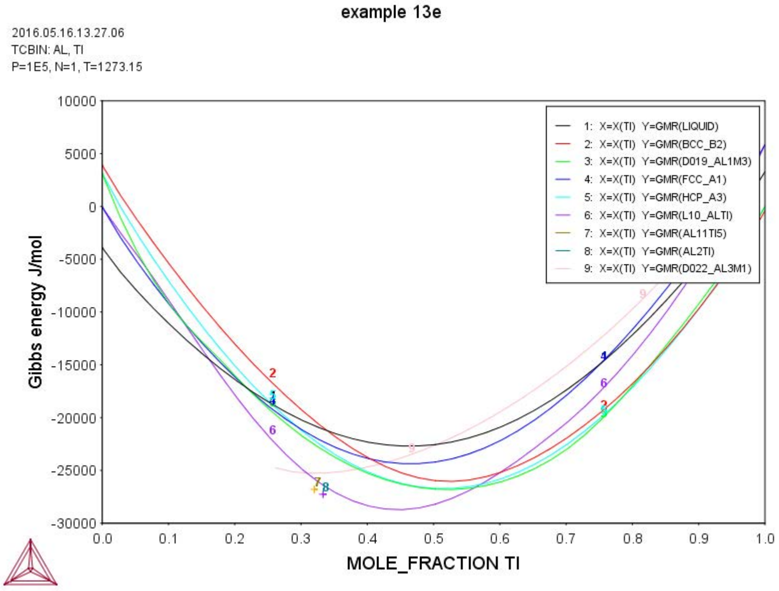


```
POST:
POST:Hit RETURN to continue
POST: @@ Now the G curves for the same system
POST: BA
   ... the command in full is BACK
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
SYS: GO BIN
   ... the command in full is GOTO_MODULE
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC Binary Solutions  v1.1

 VA                       /-  DEFINED
 BCC_B2                   FCC_L12                  FCC_L102
 D021_HCP  REJECTED
First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G
Temperature (C): /1000/: 1000
   ... the command in full is REJECT
 VA                       /-  DEFINED
 BCC_B2                   FCC_L12                  FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
```

```
AL                      TI  DEFINED
GAS:G                   LIQUID:L                IONIC_LIQUID:Y
FCC_A1                  BCC_A2                  A2_BCC
HCP_A3                  HCP_ZN                  DIAMOND_A4
BCT_A5                  CBCC_A12                CUB_A13
B11_CUTI                B32_ALLI                C14_LAVES
C15_LAVES               C16_AL2CU               C36_LAVES
D019_AL1M3              D019_SNTI3              D022_AL3M1
D1A_CU4TI               D513_AL3NI2             D88_SI3TI5
L10_ALTI                AL11TI5                 AL2TI
AL5FE4                  ALCE_AMORPHOUS          MTI2
  REJECTED
LIQUID:L  RESTORED
AL11TI5  RESTORED
AL2TI  RESTORED
D022_AL3M1  RESTORED
D019_AL1M3  RESTORED
L10_ALTI  RESTORED
A2_BCC  RESTORED
BCC_B2  RESTORED
FCC_A1  RESTORED
HCP_A3  RESTORED
  ... the command in full is GET_DATA
ELEMENTS .....
SPECIES ......
PHASES .......
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

 'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
 'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
 'N Saunders, COST 507 (1998) ISBN 92-828-3902-8 p 89-94; Al-Ti'
 'N. Dupin, 1999, lattice stability for G(BCC_A2,VA:VA)'
 'N. Dupin, I. Ansara, Z. metallkd., Vol 90 (1999) p 76-85; Al-Ni'
 'A V Davydov et al, Metall Mater Trans 32A (2001)9 p 2175-2186; Co-Ti'
 'B Sundman, fix to avoid BCC with just Va (2001)'
 'B Sundman, Set to zero due to the phase partitioning model '
-OK-
  ... the command in full is SET_AXIS_VARIABLE
The condition X(TI)=.1234  created
  ... the command in full is SET_CONDITION
  ... the command in full is COMPUTE_EQUILIBRIUM
  ... the command in full is SET_REFERENCE_STATE
  ... the command in full is SET_REFERENCE_STATE
  ... the command in full is SAVE_WORKSPACES
  ... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
  ... the command in full is COMPUTE_EQUILIBRIUM
  ... the command in full is COMPUTE_EQUILIBRIUM
  ... the command in full is SAVE_WORKSPACES
  ... the command in full is STEP_WITH_OPTIONS

Phase Region from   0.502463     for:
    LIQUID
    BCC_B2
    D019_AL1M3
    FCC_A1
    HCP_A3
    L10_ALTI

Phase Region from   0.502463     for:
    LIQUID
    BCC_B2
    D019_AL1M3
    FCC_A1
    HCP_A3
    L10_ALTI

Phase Region from   0.320000     for:
    AL11TI5

Phase Region from   0.333333     for:
    AL2TI

Phase Region from   0.636878     for:
    D022_AL3M1

Phase Region from   0.636878     for:
    D022_AL3M1
*** Buffer saved on file ***
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex13\GCUR
VE.POLY3

 POSTPROCESSOR VERSION 3.2

  ... the command in full is SET_TIELINE_STATUS
  ... the command in full is SET_LABEL_CURVE_OPTION
  ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-label F
  ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13e
POST:
POST: plot
  ... the command in full is PLOT_DIAGRAM
```

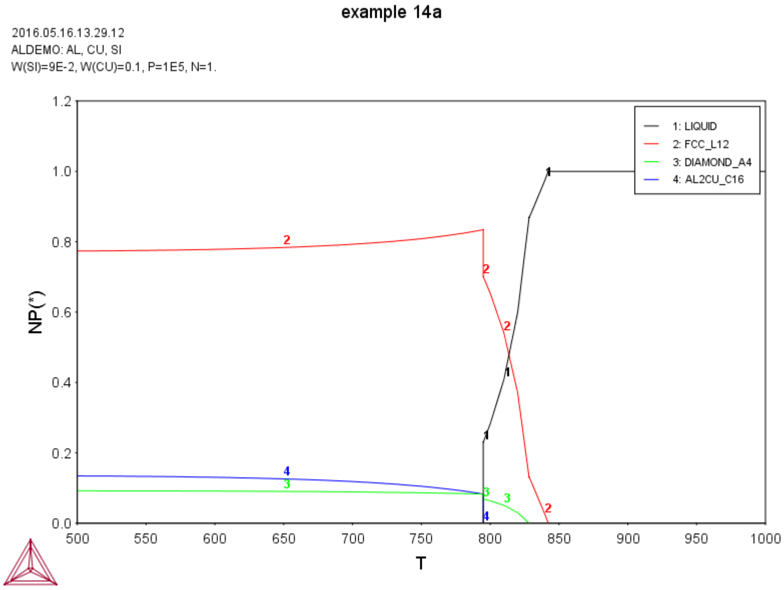


```
POST:
POST: set-inter
  ... the command in full is SET_INTERACTIVE_MODE
POST:
```

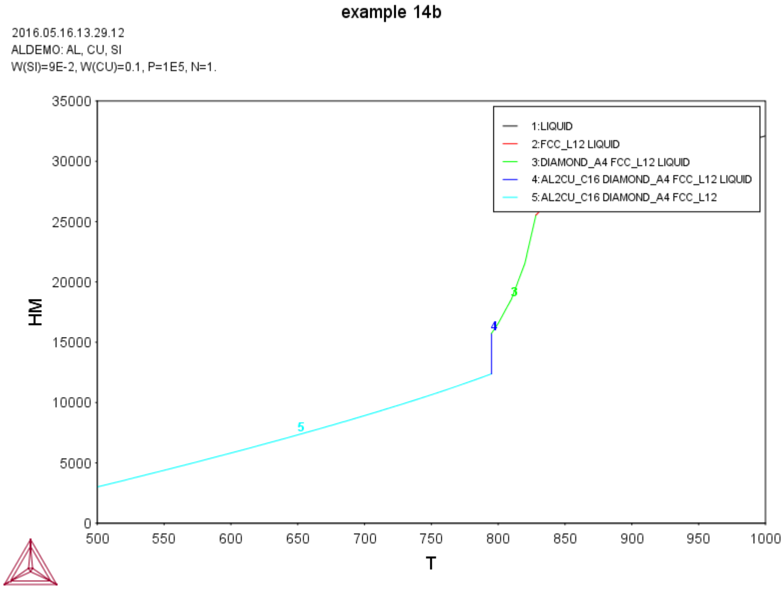
tcex14

```
About License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex14\tcex14.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of the variation of the heat and the heat capacity
SYS: @@ during solidification of an Al-Cu-Si alloy
SYS: @@
SYS: set-log ex14,,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw ALDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Aluminum Demo Database

 VA                       /-  DEFINED
TDB_ALDEMO: d-sys al cu si
   ... the command in full is DEFINE_SYSTEM
 AL                       CU                       SI
   DEFINED
TDB_ALDEMO: l-s c
   ... the command in full is LIST_SYSTEM
 LIQUID      :AL CU SI:
 HCP_A3      :AL CU SI:VA:
 BCC_A2      :AL CU SI:VA:
 BCC_B2      :AL CU SI:AL CU SI:VA:
 FCC_A1      :AL CU SI:VA:
 FCC_L12     :AL CU SI:AL CU SI:VA:
 C14_LAVES   :AL CU:AL CU:
 DIAMOND_A4  :AL SI:
 C15_LAVES   :AL CU SI:AL CU SI:
 C36_LAVES   :AL CU:AL CU:
 AL2CU_C16   :AL:AL CU SI:
 ALCU_DEL    :AL:CU:
 ALCU_EPS    :AL CU:CU:
 ALCU_ETA    :AL CU:CU:
 ALCU_PRIME  :AL:CU:
 ALCU_ZETA   :AL:CU:
 GAMMA_D83   :AL SI:AL CU SI:CU:
 GAMMA_H     :AL:AL CU:CU:
 CU15SI4_EPSILON :CU:AL SI:
 CU33SI7_DELTA :CU:SI:
 CU56SI11_GAMMA :CU SI:SI:
 CUSI_ETA    :CU:SI:
TDB_ALDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, Calphad, 15 (1991) 317-425; unary data'
  'Volume data from TCFE4, 2006'
  'X.-G. Lu, et al., CALPHAD, 29 (2005) 68-89; Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, 2006; Molar volumes'
  'I. Ansara (Editor), COST 507, (1998)'
  'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),CU-Si'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'
  'C.-Y. He,Calphad, 33,200-210 (2009),Al-Cu-Si'
  'Volume data, N. Dupin 2008'
  'L. Kjellqvist, Thermo-Calc Software AB, 2010; Unassessed parameter,
      linear combination of unary volume data'
  'Hai-Lin Chen, in TCAL2.0, Extrapolations, assumptions
       adjustment'
  'J.R.Zhao, Y.Du, in , 2010, Sn-Sr, Cu-Mg-Si'
  'L. Kjellqvist, Thermo-Calc Software AB, 2012; Molar volumes'
  'W.H. Sun,unpublished (2010),Cu-Si-Zn,Cu-Ni-Zn'
 -OK-
TDB_ALDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ The composition
POLY_3: s-c w(si)=.09,w(cu)=.10,t=1000,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(SI)=9E-2, W(CU)=0.1, T=1000, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16528 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: ALDEMO

 Conditions:
 W(SI)=9E-2, W(CU)=0.1, T=1000, P=1E5, N=1
 DEGREES OF FREEDOM 0
```

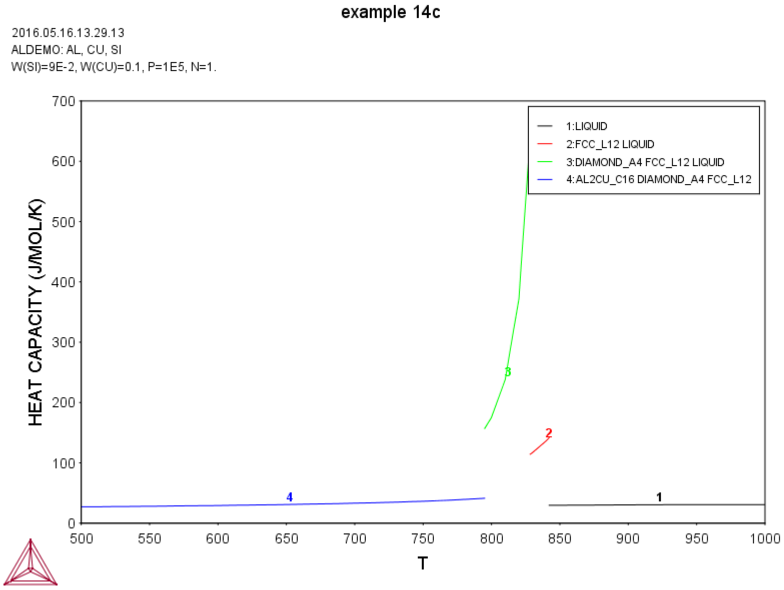
```
 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.87371E+01
 Total Gibbs energy -4.64558E+04,  Enthalpy  3.21074E+04,  Volume  1.02742E-05

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      8.6269E-01  8.1000E-01 5.0275E-03 -4.4007E+04 SER
 CU                      4.5223E-02  1.0000E-01 3.2656E-06 -1.0503E+05 SER
 SI                      9.2090E-02  9.0000E-02 7.5475E-03 -4.0629E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.8737E+01, Volume fraction 1.0000E+00  Mass fractions:
 AL  8.10000E-01  CU  1.00000E-01  SI  9.00000E-02
POLY_3:Hit RETURN to continue
POLY_3: @@ Set termperature as axis
POLY_3: s-a-v
   ... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: t
Min value /0/: 500
Max value /1/: 1000
Increment /12.5/: 12.5
POLY_3: save tcex14 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   1000.000
...OK

 Phase Region from   1000.000     for:
     LIQUID
 Global test at  9.20000E+02 .... OK
 Global check of adding phase at  8.42133E+02
 Calculated    18 equilibria

 Phase Region from    842.133     for:
     FCC_L12
     LIQUID
 Global check of adding phase at  8.28227E+02
 Calculated     5 equilibria

 Phase Region from    828.227     for:
     DIAMOND_A4
     FCC_L12
     LIQUID
 Global check of adding phase at  7.94999E+02
 Calculated     6 equilibria

 Phase Region from    794.999     for:
     AL2CU_C16
     DIAMOND_A4
     FCC_L12
     LIQUID
 Calculated     2 equilibria

 Phase Region from    794.999     for:
     AL2CU_C16
     DIAMOND_A4
     FCC_L12
 Global test at  7.20000E+02 .... OK
 Global test at  6.20000E+02 .... OK
 Global test at  5.20000E+02 .... OK
 Terminating at    500.000
 Calculated    33 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex14\tcex
 14.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: @@ Plot phase fractions
POST: S-D-A X T
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y NP(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: S-LAB D
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 14a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the total enthalpy (heat)
POST: S-D-A Y HM
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-LAB B
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 14b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the heat capacity. This must first be entered as
POST: @@ a function as derivatives cannot be plotted directly.
POST: ENT FUN CP=HM.T;
   ... the command in full is ENTER_SYMBOL
POST: S-D-A Y CP
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-S
   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC SCALING  (Y OR N) /N/: N
MIN VALUE : 0
MAX VALUE : 700
POST: S-A-T-S
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC AXIS TEXT  (Y OR N) /N/: N
AXIS TEXT : HEAT CAPACITY (J/MOL/K)
POST: set-title example 14c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



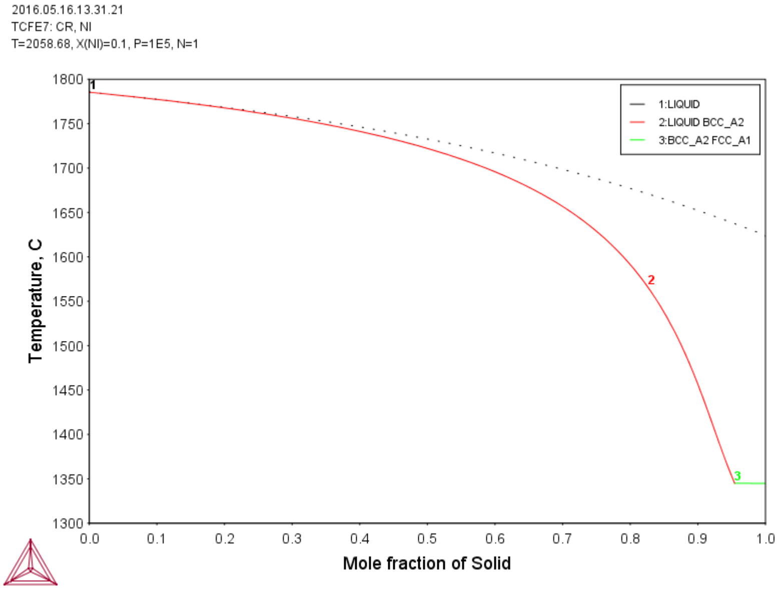
```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex15

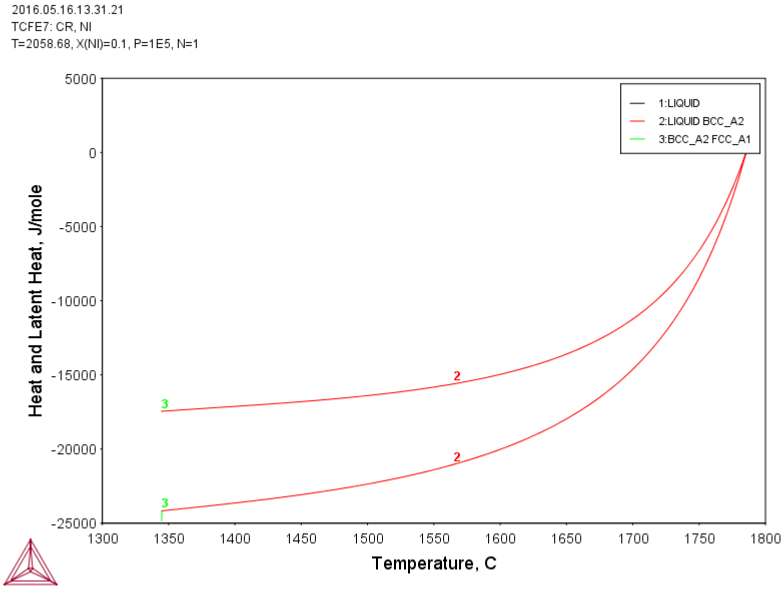
```
About Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex15\tcex15.TCM"SYS: SET_ECHO
SYS: @@
SYS: @@
SYS: @@ This is an example of a solidification simulation of a Cr-Ni alloy.
SYS: @@ No back diffusion in the solid, i.e. Scheil-Gulliver model.
SYS: @@
SYS: SET-LOG ex15,,,
SYS: GO SCHEIL
   ... the command in full is GOTO_MODULE
SCHEIL: TEMPERATURE-STEP
Temperature step (C) /1/: 5
SCHEIL: START-WIZARD
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: TCFE7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: cr
Composition input in mass (weight) percent? /Y/: n
 Composition will be taken to be in mole percent
1st alloying element: ni
Mole percent /1/: 10
2nd alloying element:
Temperature (C) /2000/: 2000
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED


 This database has following phases for the defined system

 LIQUID:L                 BCC_A2                   FCC_A1
 HCP_A3                   SIGMA                    CHI_A12
 LAVES_PHASE_C14          CR3SI                    NBNI3
 NI3TI

Reject phase(s) /NONE/: *
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  SIGMA                   CHI_A12
 LAVES_PHASE_C14         CR3SI                   NBNI3
 NI3TI  REJECTED
Restore phase(s):: liq bcc fcc
 LIQUID:L                BCC_A2                  FCC_A1
   RESTORED
Restore phase(s): /NONE/: NONE

 ........................................................

    The following phases are retained in this system:

 LIQUID:L                 BCC_A2                   FCC_A1

 ........................................................

OK? /Y/: y
 GAS:G  REJECTED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, pp. 1155-1170'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
 -OK-
Should any phase have a miscibility gap check? /N/:
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/:
   ... the command in full is SET_NUMERICAL_LIMITS
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=2273.15, X(NI)=0.1, P=1E5, N=1    DEGREES OF FREEDOM 0
To form BCC_A2#1 the condition is set to T=2058.59460117
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
   ... the command in full is ADVANCED_OPTIONS
   ... the command in full is STEP_WITH_OPTIONS
...OK

 Phase Region from    2058.58     for:
     LIQUID
     BCC_A2
 Global check of removing phase at  2.05859E+03
 Calculated     3 equilibria
```

```
Phase Region from    2058.59     for:
    LIQUID
Terminating at    2058.68
Calculated     4 equilibria

Phase Region from    2058.58     for:
    LIQUID
    BCC_A2
Global test at  2.01858E+03 .... OK
Global test at  1.96858E+03 .... OK
Global test at  1.91858E+03 .... OK
Global check of removing phase at  1.89734E+03
Calculated    35 equilibria

Phase Region from    1897.34     for:
    BCC_A2
Calculated     4 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex15\SCHE
IL_4176.POLY3

 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes


 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes

  ... the command in full is ENTER_SYMBOL
  ... the command in full is MAKE_EXPERIMENTAL_DATAFI
An EXP file c:\jenkins\WORKSP~1\THERMO~1\examples\tcex15\SCHEIL_EQ_4176.EXP
has been created to store the equilibrium solidification results.
  ... the command in full is READ_WORKSPACES
 CALCULATING SCHEIL SOLIDFICATION
  ... the command in full is SET_NUMERICAL_LIMITS

    T(C)      fraction solid

  1785.535       0.000000

 PHASE REGION:LIQUID + BCC_A2

    T(C)      fraction solid

  1785.378      0.8823747E-03
  1780.378      0.6490648E-01
  1775.378      0.1226306
  1770.378      0.1748823
  1765.378      0.2223552
  1760.378      0.2656343
  1755.378      0.3052160
  1750.378      0.3415242
  1745.378      0.3749225
  1740.378      0.4057245
  1735.378      0.4342018
  1730.378      0.4605909
  1725.378      0.4850982
  1720.378      0.5079050
  1715.378      0.5291708
  1710.378      0.5490363
  1705.378      0.5676264
  1700.378      0.5850522
  1695.378      0.6014127
  1690.378      0.6167963
  1685.378      0.6312824
  1680.378      0.6449423
  1675.378      0.6578403
  1670.378      0.6700345
  1665.378      0.6815775
  1660.378      0.6925168
  1655.378      0.7028958
  1650.378      0.7127541
  1645.378      0.7221276
  1640.378      0.7310493
  1635.378      0.7395494
  1630.378      0.7476556
  1625.378      0.7553933
  1620.378      0.7627859
  1615.378      0.7698550
  1610.378      0.7766207
  1605.378      0.7831013
  1600.378      0.7893139
  1595.378      0.7952744
  1590.378      0.8009975
  1585.378      0.8064969
  1580.378      0.8117854
  1575.378      0.8168749
  1570.378      0.8217764
  1565.378      0.8265005
  1560.378      0.8310568
  1555.378      0.8354544
  1550.378      0.8397021
  1545.378      0.8438078
  1540.378      0.8477792
  1535.378      0.8516235
  1530.378      0.8553475
  1525.378      0.8589580
  1520.378      0.8624606
  1515.378      0.8658613
  1510.378      0.8691657
  1505.378      0.8723790
  1500.378      0.8755064
  1495.378      0.8785528
  1490.378      0.8815228
  1485.378      0.8844210
  1480.378      0.8872519
  1475.378      0.8900197
  1470.378      0.8927287
  1465.378      0.8953829
  1460.378      0.8979866
  1455.378      0.9005436
```

```
  1450.378      0.9030572
  1445.378      0.9055331
  1440.378      0.9079746
  1435.378      0.9103858
  1430.378      0.9127710
  1425.378      0.9151344
  1420.378      0.9174805
  1415.378      0.9198139
  1410.378      0.9221392
  1405.378      0.9244614
  1400.378      0.9267856
  1395.378      0.9291170
  1390.378      0.9314612
  1385.378      0.9338239
  1380.378      0.9362111
  1375.378      0.9386289
  1370.378      0.9410835
  1365.378      0.9435813
  1360.378      0.9461287
  1355.378      0.9487319
  1350.378      0.9513970
  1345.378      0.9541295
  1344.910      0.9543771

 PHASE REGION:BCC_A2 + FCC_A1

    T(C)      fraction solid

  1344.753      1.0000000

Hint: move the last function to the first equilibrium where it is used

  ... the command in full is SET_LABEL_CURVE_OPTION
  ... the command in full is APPEND_EXPERIMENTAL_DATA
```



```
  ... the command in full is APPEND_EXPERIMENTAL_DATA

 ...........................................................

       The following axis variables are available

            T --- Temperature in Celsius
        NL/BL --- Mole/mass fraction of liquid
        NS/BS --- Mole/mass fraction of all solid phases
NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
     W(ph,el) --- Weight fraction of an element in a phase
     X(ph,el) --- Mole fraction of an element in a phase
     Y(ph,el) --- Site fraction of an element in a phase
    NN(ph,el) --- Distribution of an element in a phases
        NH/BH --- Heat release and Latent heat per mole/gram
       CP/BCP --- Apparent heat capacity per mole/gram
    NV/NV(ph) --- Molar volume of the system or a phase
    DS/DS(ph) --- Average density of the system or a phase
           BT --- Apparent volumetric TEC of the system

 "el" and "ph" are name of element and phase, respectively
    "*" can be used as a wild character for "el" and "ph"

 ..........................................................

POST: s-d-a x t
  ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y nh
  ... the command in full is SET_DIAGRAM_AXIS
POST: plot,,,,,,,,,,
  ... the command in full is PLOT_DIAGRAM
```



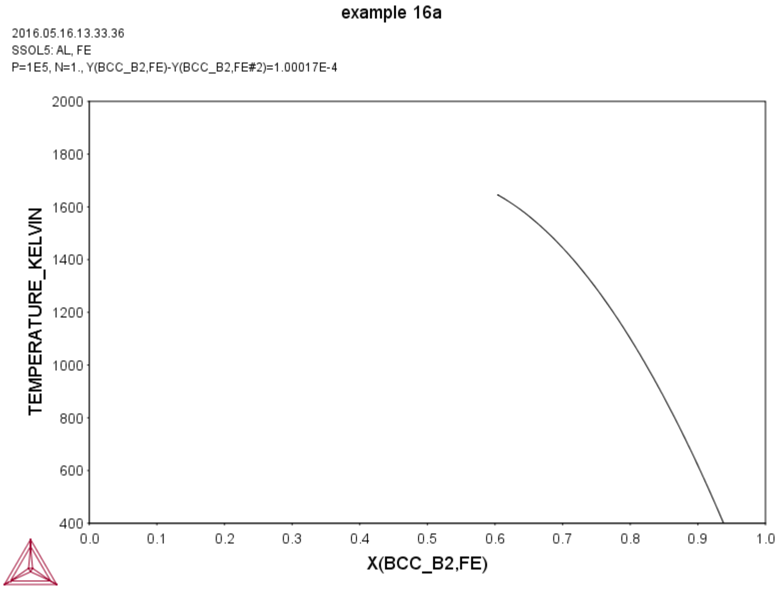
```
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex16

```
About simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex16\tcex16.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of the second order transition line in the Bcc field of the Al-Fe system
SYS: @@
SYS: SET-LOG ex16,,
SYS: GO DA
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: SW SSOL5
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Alloy Solutions Database v5.0

 VA  DEFINED
 GAS:G  REJECTED
TDB_SSOL5: D-SYS AL FE
   ... the command in full is DEFINE_SYSTEM
 AL                      FE  DEFINED
TDB_SSOL5: REJ PH /ALL
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  FCC_L12
 BCC_A2                  BCC_B2                  B2_BCC
 HCP_A3                  HCP_ZN                  DHCP
 DIAMOND_A4              BCT_A5                  TETRAGONAL_U
 CBCC_A12                CUB_A13                 ORTHORHOMBIC_A20
 RHOMBO_C19              LAVES_C14               LAVES_C15
 LAVES_C36               M4N                     ALM_D019
 ALCE_AMORPHOUS          ALCU_THETA              AL2FE
 AL5FE2                  AL5FE4                  AL13FE4
 ALLI                    AL4MN                   AL6MN
 AL11MN4                 AL12MN                  ALNB3
 AL3NB                   AL3NI2                  ALPT3
 ALTI                    CR3SI_A15               D_GAMMA
 FEPD                    FEPD3                   FESB
 FEU6                    FE2U                    FEZN_GAMMA_D82
 FEZN4                   FEZN_DELTA              FEZN_ZETA
 FEUZR_DELTA             FEZR2                   FEZR3
   REJECTED
TDB_SSOL5: @@ The BCC phase has B2 ordering in this system
TDB_SSOL5: @@ Note that this is modelled with two sublattices
TDB_SSOL5: @@ with both components in both sublattices
TDB_SSOL5: REST PH LIQ BCC_B2 BCC_A2
   ... the command in full is RESTORE
 LIQUID:L                BCC_B2                  BCC_A2
   RESTORED
TDB_SSOL5: LI-SYS
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 LIQUID:L    :AL FE:
 BCC_A2      :AL FE:VA:
 BCC_B2      :AL FE:AL FE:VA:
TDB_SSOL5: GET
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Data for the Al-Fe system were from an unpublished assessment of M
      Seiersten published in the COST507 final report: COST507
      Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,
       AT Dinsdale and MH Rand, July 1998, EUR18499. >> Al-Fe '
 -OK-
TDB_SSOL5: GO P-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3:
POLY_3: advanced global_minimization y 10000
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY_3:
POLY_3: @@ Set conditions where the BCC phase should be ordered
POLY_3: SET-COND P=1E5,N=1,T=400,X(AL)=.4
   ... the command in full is SET_CONDITION
POLY_3: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         10065 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ Use option N in order to see how Al and Fe distribute
POLY_3: @@ on the sublattices
POLY_3: LIST-EQ
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: N
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL5
```

```
 Conditions:
 P=1E5, N=1, T=400, X(AL)=0.4
 DEGREES OF FREEDOM 0

 Temperature    400.00 K (   126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.43010E+01
 Total Gibbs energy -3.81486E+04,  Enthalpy -2.55850E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      4.0000E-01  2.4362E-01 4.1973E-08 -5.6493E+04 SER
 FE                      6.0000E-01  7.5638E-01 4.1248E-04 -2.5919E+04 SER

 BCC_B2                   ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.4301E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  7.56376E-01  AL  2.43624E-01
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  9.99996E-01  AL  4.22881E-06
 Sublattice  2,  Number of sites  5.0000E-01
 AL  7.99996E-01  FE  2.00004E-01
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Change the condition of Al amount to be that the site-fractions
POLY_3: @@ in the two sublattices will have a certain difference. If they
POLY_3: @@ are the same the BCC phase is disordered
POLY_3: SET-COND X(AL)=NONE
   ... the command in full is SET_CONDITION
POLY_3: SET-COND Y(BCC_B2,FE#1)-Y(BCC_B2,FE#2)=0.1
   ... the command in full is SET_CONDITION
POLY_3: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    26 ITS,  CPU TIME USED   0 SECONDS
POLY_3: LIST-EQ
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/:Hit RETURN to continue
Options /VWNS/: @@ Set the difference smaller. This is as close to the second order
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL5

 Conditions:
 P=1E5, N=1, T=400, Y(BCC_B2,FE)-Y(BCC_B2,FE#2)=0.1
 DEGREES OF FREEDOM 0

 Temperature    400.00 K (   126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.36842E+01
 Total Gibbs energy -1.86969E+04,  Enthalpy -4.69474E+03,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      7.4926E-02  3.7658E-02 7.3790E-14 -1.0056E+05 SER
 FE                      9.2507E-01  9.6234E-01 2.6569E-02 -1.2066E+04 SER

 BCC_B2                   ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3684E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.62342E-01  AL  3.76585E-02
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  9.75074E-01  AL  2.49265E-02
 Sublattice  2,  Number of sites  5.0000E-01
 FE  8.75074E-01  AL  1.24926E-01
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3: @@ transition as it is possible to be
POLY_3: SET-COND Y(BCC_B2,FE#1)-Y(BCC_B2,FE#2)=1E-4
   ... the command in full is SET_CONDITION
POLY_3: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    14 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Now vary the temperature using these conditions
POLY_3: SET-AXIS-VAR 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: T
Min value /0/: 400
Max value /1/: 2000
Increment /40/: 10
POLY_3: @@ Always save before STEP or MAP (unless you want to overlay the new
POLY_3: @@ results on some previous results)
POLY_3: SAVE tcex16 Y
   ... the command in full is SAVE_WORKSPACES
POLY_3: STEP NORMAL
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    400.000
...OK

 Phase Region from    400.000     for:
     BCC_B2
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
 Global test at  1.28000E+03 .... OK
 Global test at  1.38000E+03 .... OK
 Global test at  1.48000E+03 .... OK
 Global test at  1.58000E+03 .... OK
 Global check of adding phase at  1.64515E+03
 Calculated   127 equilibria

 Phase Region from    1645.15     for:
     LIQUID
     BCC_B2
 Global check of removing phase at  1.64515E+03
 Calculated     3 equilibria
```

```
 Phase Region from    1645.15     for:
     BCC_B2
 Global check of adding phase at  1.64515E+03
 Calculated      3 equilibria

 Phase Region from    1645.15     for:
     LIQUID
     BCC_B2
 Calculated      3 equilibria
 Sorry cannot continue      0 189 1    1.6451539E+03
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex16\tcex
 16.POLY3
POLY_3: POST

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: SET-DIA-AXIS X X(BCC_B2,FE)
   ... the command in full is SET_DIAGRAM_AXIS
POST: SET-DIA-AXIS Y T-K
   ... the command in full is SET_DIAGRAM_AXIS
POST: SET-SCAL X N 0 1
   ... the command in full is SET_SCALING_STATUS
POST: SET-SCAL Y N 400 2000
   ... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 16a
POST: PLOT
   ... the command in full is PLOT_DIAGRAM
```



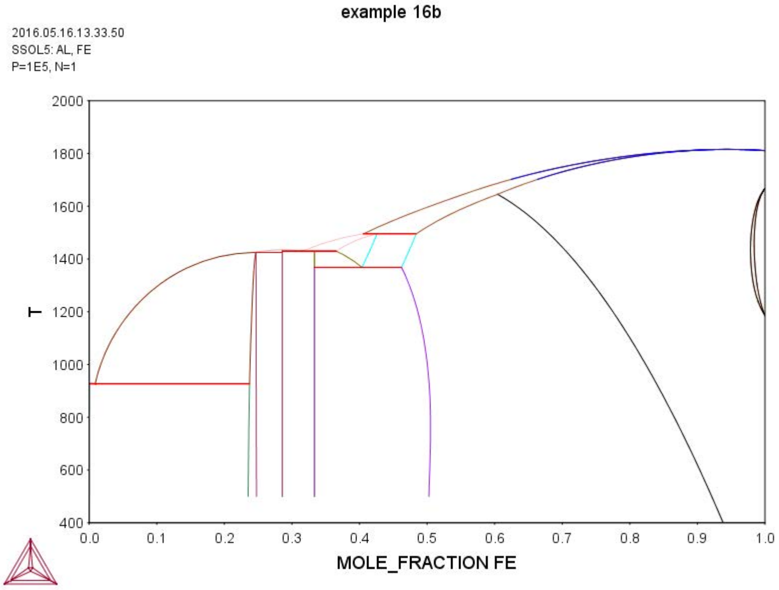
```
POST:
POST:Hit RETURN to continue
POST: @@ Write on file for plotting together with phase diagram
POST: MAKE TCEX16
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: Y
  No such command, use HELP
POST: BACK
POLY_3: GO DA
   ... the command in full is GOTO_MODULE
TDB_SSOL5: @@ Get data for all phases stable in Al-Fe
TDB_SSOL5: REJ-SYS
   ... the command in full is REJECT
 VA   DEFINED
 GAS:G  REJECTED
 REINITIATING GES5 .....
TDB_SSOL5: D-SYS AL FE
   ... the command in full is DEFINE_SYSTEM
 AL                       FE   DEFINED
TDB_SSOL5: L-SYS
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENT
 LIQUID:L     :AL FE:
 FCC_A1       :AL FE:VA:
 FCC_L12      :AL FE:AL FE:VA:
 BCC_A2       :AL FE:VA:
 BCC_B2       :AL FE:AL FE:VA:
 B2_BCC       :AL:VA:
 HCP_A3       :AL FE:VA:
 HCP_ZN       :AL:VA:
 DHCP         :AL:
 DIAMOND_A4   :AL:
 BCT_A5       :AL:
 TETRAGONAL_U :FE:
 CBCC_A12     :AL FE:VA:
 CUB_A13      :AL FE:VA:
 ORTHORHOMBIC_A20 :FE:
 RHOMBO_C19   :AL:
 LAVES_C14    :AL FE:AL FE:
 LAVES_C15    :AL FE:AL FE:
 LAVES_C36    :AL:AL:
 M4N          :FE:VA:
 ALM_D019     :AL:AL:
 ALCE_AMORPHOUS :AL:
 ALCU_THETA   :AL:AL:
 AL2FE        :AL:FE:
 AL5FE2       :AL:FE:
 AL5FE4       :AL FE:
 AL13FE4      :AL:FE:AL VA:
```

```
 ALLI        :AL:VA:
 AL4MN       :AL:FE:
 AL6MN       :AL:FE:
 AL11MN4     :AL:FE:
 AL12MN      :AL:FE:
 ALNB3       :AL:AL:
 AL3NB       :AL:AL:
 AL3NI2      :AL:AL:VA:
 ALPT3       :AL:AL:
 ALTI        :AL:AL:
 CR3SI_A15   :FE:AL:VA:
 D_GAMMA     :AL:
 FEPD        :FE:FE:
 FEPD3       :FE:FE:
 FESB        :FE:FE:
 FEU6        :FE:FE:
 FE2U        :FE:FE:
 FEZN_GAMMA_D82 :FE:FE:
 FEZN4       :FE:FE:
 FEZN_DELTA  :FE:FE:
 FEZN_ZETA   :FE:FE:
 FEUZR_DELTA :FE:FE:
 FEZR2       :FE:FE:
 FEZR3       :FE:FE:
TDB_SSOL5: REJ PH /ALL
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  FCC_L12
 BCC_A2                  BCC_B2                  B2_BCC
 HCP_A3                  HCP_ZN                  DHCP
 DIAMOND_A4              BCT_A5                  TETRAGONAL_U
 CBCC_A12                CUB_A13                 ORTHORHOMBIC_A20
 RHOMBO_C19              LAVES_C14               LAVES_C15
 LAVES_C36               M4N                     ALM_D019
 ALCE_AMORPHOUS          ALCU_THETA              AL2FE
 AL5FE2                  AL5FE4                  AL13FE4
 ALLI                    AL4MN                   AL6MN
 AL11MN4                 AL12MN                  ALNB3
 AL3NB                   AL3NI2                  ALPT3
 ALTI                    CR3SI_A15               D_GAMMA
 FEPD                    FEPD3                   FESB
 FEU6                    FE2U                    FEZN_GAMMA_D82
 FEZN4                   FEZN_DELTA              FEZN_ZETA
 FEUZR_DELTA             FEZR2                   FEZR3
   REJECTED
TDB_SSOL5: REST PH LIQ BCC_B2 FCC_A1 BCC_A2 AL13FE4 AL2FE AL5FE2 AL5FE4
   ... the command in full is RESTORE
 LIQUID:L                BCC_B2                  FCC_A1
 BCC_A2                  AL13FE4                 AL2FE
 AL5FE2                  AL5FE4  RESTORED
TDB_SSOL5: GET
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Data for the Al-Fe system were from an unpublished assessment of M
      Seiersten published in the COST507 final report: COST507
      Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,
       AT Dinsdale and MH Rand, July 1998, EUR18499. >> Al-Fe '
 -OK-
TDB_SSOL5: GO P-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ Calculate an equilibrium where BCC is ordered
POLY_3: S-C T=1300,P=1E5,N=1,X(AL)=.3
   ... the command in full is SET_CONDITION
POLY_3: C-E
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         10478 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ List the equilibrium. Note that option N gives the
POLY_3: @@ constitution of the BCC phase and this shows that the
POLY_3: @@ site-fractions are different in the two sublattices,
POLY_3: @@ i.e. the BCC is ordered
POLY_3: L-E
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/: N
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL5

 Conditions:
 T=1300, P=1E5, N=1, X(AL)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1300.00 K (  1026.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.71875E+01
 Total Gibbs energy -8.63003E+04,  Enthalpy  1.26381E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      3.0000E-01  1.7154E-01 3.1606E-05 -1.1200E+05 SER
 FE                      7.0000E-01  8.2846E-01 9.4427E-04 -7.5285E+04 SER

 BCC_B2                   ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.7187E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.28459E-01  AL  1.71541E-01
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  8.77450E-01  AL  1.22550E-01
 Sublattice  2,  Number of sites  5.0000E-01
 FE  5.22550E-01  AL  4.77450E-01
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3:Hit RETURN to continue
```

```
POLY_3: @@ Set axis
POLY_3: S-A-V 1 X(AL)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: S-A-V 2 T
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 500
Max value /1/: 2000
Increment /37.5/: 25
POLY_3: SAVE tcex16 Y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: MAP
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Trying global minimization! 1
 Creating a new composition set BCC_B2#2
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22

 Phase region boundary   1 at:   8.364E-03  1.237E+03
     BCC_B2
  ** FCC_A1
 Calculated                     19  equilibria

 Phase region boundary   2 at:   8.364E-03  1.237E+03
     BCC_B2
  ** FCC_A1
 Calculated                     39  equilibria

 Phase region boundary   3 at:   3.562E-01  1.702E+03
  ** LIQUID
     BCC_B2
 Calculated                     35  equilibria

 Phase region boundary   4 at:   3.562E-01  1.702E+03
  ** LIQUID
     BCC_B2
 Calculated.                     16  equilibria
 Calculated                     16  equilibria

 Phase region boundary   5 at:   3.562E-01  1.702E+03
  ** LIQUID
     BCC_B2
 Calculated.                     17  equilibria

 Phase region boundary   6 at:   5.550E-01  1.496E+03
  ** LIQUID
  ** AL5FE4
     BCC_B2

 Phase region boundary   7 at:   5.452E-01  1.496E+03
  ** AL5FE4
     BCC_B2#2
 Calculated.                      7  equilibria

 Phase region boundary   8 at:   5.672E-01  1.368E+03
  ** AL2FE
  ** AL5FE4
     BCC_B2#2

 Phase region boundary   9 at:   6.023E-01  1.368E+03
  ** AL2FE
     BCC_B2#2
 Calculated..                     36  equilibria
 Terminating at axis limit.

 Phase region boundary  10 at:   6.316E-01  1.368E+03
  ** AL2FE
     AL5FE4
 Calculated.                      4  equilibria
```

```
Phase region boundary  11 at:   6.502E-01  1.428E+03
 ** AL2FE
 ** AL5FE2
    AL5FE4

Phase region boundary  12 at:   6.740E-01  1.428E+03
 ** AL5FE2
    AL5FE4
Calculated.                      2  equilibria

Phase region boundary  13 at:   6.744E-01  1.430E+03
 ** LIQUID
 ** AL5FE2
    AL5FE4

Phase region boundary  14 at:   6.593E-01  1.430E+03
 ** LIQUID
    AL5FE4
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   6.993E-01  1.430E+03
 ** LIQUID
    AL5FE2
Calculated.                     12  equilibria

Phase region boundary  16 at:   7.362E-01  1.424E+03
 ** LIQUID
 ** AL13FE4
    AL5FE2

Phase region boundary  17 at:   7.337E-01  1.424E+03
 ** AL13FE4
    AL5FE2
Calculated..                     38  equilibria
Terminating at axis limit.

Phase region boundary  18 at:   7.556E-01  1.424E+03
    LIQUID
 ** AL13FE4
Calculated.                     24  equilibria

Phase region boundary  19 at:   8.723E-01  9.271E+02
    LIQUID
 ** AL13FE4
 ** FCC_A1

Phase region boundary  20 at:   9.955E-01  9.271E+02
    LIQUID
 ** FCC_A1
Calculated                     10  equilibria

Phase region boundary  21 at:   8.813E-01  9.271E+02
    AL13FE4
 ** FCC_A1
Calculated..                     19  equilibria
Terminating at axis limit.

Phase region boundary  22 at:   6.905E-01  1.428E+03
    AL2FE
 ** AL5FE2
Calculated..                     39  equilibria
Terminating at axis limit.

Phase region boundary  23 at:   5.550E-01  1.496E+03
 ** LIQUID
    BCC_B2#2
Calculated                     50  equilibria

Phase region boundary  24 at:   5.820E-01  5.100E+02
 ** AL2FE
    BCC_B2#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  25 at:   5.820E-01  5.100E+02
 ** AL2FE
    BCC_B2#2
Calculated.                     36  equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   8.824E-01  5.100E+02
 ** AL13FE4
    FCC_A1
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  27 at:   8.824E-01  5.100E+02
 ** AL13FE4
    FCC_A1
Calculated.                     18  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   8.824E-01  5.100E+02
 ** AL13FE4
    FCC_A1
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  29 at:   8.824E-01  5.100E+02
 ** AL13FE4
    FCC_A1
Calculated.                     18  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   8.722E-01  1.003E+03
    LIQUID
 ** AL13FE4
Calculated.                      5  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   8.722E-01  1.003E+03
```

```
    LIQUID
 ** AL13FE4
Calculated.                      28  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   1.805E-02  1.497E+03
 ** BCC_B2
    FCC_A1
Calculated                      32  equilibria

Phase region boundary  33 at:   1.805E-02  1.497E+03
 ** BCC_B2
    FCC_A1
Calculated                      35  equilibria

Phase region boundary  34 at:   1.032E-02  1.813E+03
    LIQUID
 ** BCC_B2
Calculated                      13  equilibria

Phase region boundary  35 at:   1.032E-02  1.813E+03
    LIQUID
 ** BCC_B2
Calculated.                      44  equilibria
Calculated                      44  equilibria

Phase region boundary  36 at:   1.032E-02  1.813E+03
    LIQUID
 ** BCC_B2
Calculated.                      47  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   3.201E-01  1.728E+03
    LIQUID
 ** BCC_B2
Calculated                      34  equilibria

Phase region boundary  38 at:   3.201E-01  1.728E+03
    LIQUID
 ** BCC_B2
Calculated.                      19  equilibria
Calculated                      19  equilibria

Phase region boundary  39 at:   3.201E-01  1.728E+03
    LIQUID
 ** BCC_B2
Calculated.                      22  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.421E-01  1.451E+03
    LIQUID
 ** AL5FE4
Calculated.                       7  equilibria
Calculated                       7  equilibria

Phase region boundary  41 at:   6.421E-01  1.451E+03
    LIQUID
 ** AL5FE4
Calculated.                       6  equilibria
Terminating at known equilibrium

Phase region boundary  42 at:   6.421E-01  1.451E+03
    LIQUID
 ** AL5FE4
Calculated.                       3  equilibria
Terminating at known equilibrium

Phase region boundary  43 at:   8.763E-01  9.396E+02
    LIQUID
 ** AL13FE4
Calculated.                      28  equilibria
Terminating at known equilibrium

Phase region boundary  44 at:   8.763E-01  9.396E+02
    LIQUID
 ** AL13FE4
Calculated.                       2  equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex16\tcex
16.POLY3
CPU time for mapping                       7  seconds
POLY_3:
POLY_3: POST

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST: S-D-A X M-F FE
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y T
   ... the command in full is SET_DIAGRAM_AXIS
POST: @@ Append the previous line for the 2nd order transition
POST: A-E-D Y TCEX16
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 16b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
 The composition set BCC_B2#2 created from the store file
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex17

```
About Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex17\tcex17.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of the pseudo-binary system CaO-SiO2
SYS: @@ using the ionic database
SYS: @@
SYS: set-log ex17,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
TDB_TCFE8: @@ This database can be used both for pseudobinary systems like
TDB_TCFE8: @@ the one in this case, CaO-SiO2, or for full ternary systems
TDB_TCFE8: @@ like Ca-Fe-O.
TDB_TCFE8: sw OXDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Oxide Demo Database

 VA                       /-  DEFINED
TDB_OXDEMO: @@ Note that /- represent the electon.
TDB_OXDEMO: d-sys ca si o
   ... the command in full is DEFINE_SYSTEM
 CA                       SI                       O
   DEFINED
TDB_OXDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
 GAS:G       :CA CA1O1 CA2 O1SI1 O2 O2SI1 O2SI2 O3 SI SI2 SI3:
 IONIC_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 VA SIO2:
  > Ionic liquid mixture, modelled by the ionic two-sublattice model.
 BCC_A2      :CA SI:O VA:
 CA2SIO4_ALPHA :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2. Prototype Ca2[SiO4] (hP24, P63/mmc)
 CA2SIO4_ALPHA_PRIME:I :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2. Prototype Sr2[SiO4] (oP52, Pnma)
 CRISTOBALITE :SIO2:
  > Prototype SiO2 (cF24, Fd3m)
 DIAMOND_FCC_A4 :SI:O VA:
  > Silicon (cF8, Fd-3m)
 FCC_A1      :CA SI:O VA:
 HALITE:I    :CA+2 VA:O-2:
  > This is CaO and FeO (cI2, Im-3m)
 HATRURITE   :CA+2:SI+4:O-2:
  > This is 3CaO.SiO2 (hR81, R3m)
 HCP_A3      :CA SI:VA:
 LARNITE     :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 (metastable at 1 atm)
 OLIVINE:I   :CA+2:CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 and fayalite
 PSEUDO_WOLLASTONITE :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (mS120, C12/c1)
 QUARTZ      :SIO2:
  > Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))
 RANKINITE   :CA+2:SI+4:O-2:
  > This is 3CaO.2SiO2 (mP48, P121/c1)
 TRIDYMITE   :SIO2:
  > Prototype SiO2 (hP12, P63/mmc)
 WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (aP30, P-1)
TDB_OXDEMO: @@ If we want to calculate a pseudobinary system
TDB_OXDEMO: @@ we must take away all phases and constituents that make it
TDB_OXDEMO: @@ possible for the phase to exist outside the composition line
TDB_OXDEMO: @@ from CaO to SiO2.
TDB_OXDEMO: @@ This means that for the IONIC_LIQ phase the constituent Va should
TDB_OXDEMO: @@ be suspended for systems with no degree of freedom with
TDB_OXDEMO: @@ respect to oxygen
TDB_OXDEMO: rej const
   ... the command in full is REJECT
PHASE: ion
SUBLATTICE NUMBER: 2
CONSTITUENT: va
 VA IN IONIC_LIQ:Y SUBLATTICE   2 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
 GAS:G       :CA CA1O1 CA2 O1SI1 O2 O2SI1 O2SI2 O3 SI SI2 SI3:
 IONIC_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 SIO2:
  > Ionic liquid mixture, modelled by the ionic two-sublattice model.
 BCC_A2      :CA SI:O VA:
 CA2SIO4_ALPHA :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2. Prototype Ca2[SiO4] (hP24, P63/mmc)
 CA2SIO4_ALPHA_PRIME:I :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2. Prototype Sr2[SiO4] (oP52, Pnma)
 CRISTOBALITE :SIO2:
  > Prototype SiO2 (cF24, Fd3m)
 DIAMOND_FCC_A4 :SI:O VA:
  > Silicon (cF8, Fd-3m)
 FCC_A1      :CA SI:O VA:
 HALITE:I    :CA+2 VA:O-2:
  > This is CaO and FeO (cI2, Im-3m)
 HATRURITE   :CA+2:SI+4:O-2:
  > This is 3CaO.SiO2 (hR81, R3m)
 HCP_A3      :CA SI:VA:
 LARNITE     :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 (metastable at 1 atm)
 OLIVINE:I   :CA+2:CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 and fayalite
 PSEUDO_WOLLASTONITE :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (mS120, C12/c1)
 QUARTZ      :SIO2:
```

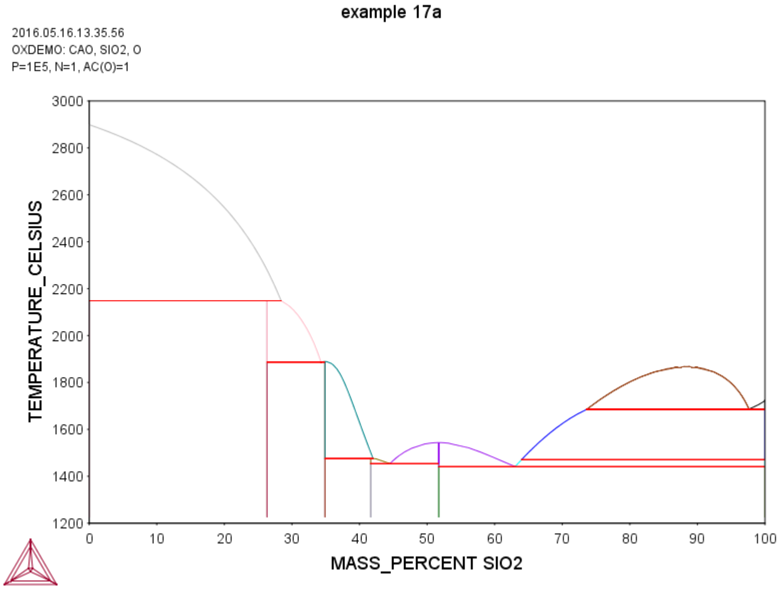
```
  > Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))
 RANKINITE   :CA+2:SI+4:O-2:
  > This is 3CaO.2SiO2 (mP48, P121/c1)
 TRIDYMITE   :SIO2:
  > Prototype SiO2 (hP12, P63/mmc)
 WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (aP30, P-1)
TDB_OXDEMO:Hit RETURN to continue
TDB_OXDEMO: @@ The phase names may seem unfamiliar but this is due to the
TDB_OXDEMO: @@ attempt to create a general database. Thus lime (CaO) is
TDB_OXDEMO: @@ called HALITE which is the generic phase name for this structure.
TDB_OXDEMO: @@ HALITE is also the wudstite phase (FeO) and the periclase phase (MgO)
TDB_OXDEMO: @@ Note also that many phases are modelled with sublattices and
TDB_OXDEMO: @@ vacancies in order to allow for non-stoichiometry in higher
TDB_OXDEMO: @@ order system.
TDB_OXDEMO: @@ For simplicity we reject all phases except those we know
TDB_OXDEMO: @@ should be stable in this system.
TDB_OXDEMO: @@
TDB_OXDEMO: rej ph /all
   ... the command in full is REJECT
 GAS:G                   IONIC_LIQ:Y             BCC_A2
 CA2SIO4_ALPHA           CA2SIO4_ALPHA_PRIME:I   CRISTOBALITE
 DIAMOND_FCC_A4          FCC_A1                  HALITE:I
 HATRURITE               HCP_A3                  LARNITE
 OLIVINE:I               PSEUDO_WOLLASTONITE     QUARTZ
 RANKINITE               TRIDYMITE               WOLLASTONITE:I
   REJECTED
TDB_OXDEMO: rest ph ionic_liq alpha_ca2sio4 alpha_prime cristobalite halite hatrurite
   ... the command in full is RESTORE
 *** ALPHA_CA2SIO4 INPUT IGNORED
 *** ALPHA_PRIME INPUT IGNORED
 IONIC_LIQ:Y             CRISTOBALITE            HALITE:I
 HATRURITE  RESTORED
TDB_OXDEMO: rest ph larnite olivine pseudo_wollastonite quartz rankinite
   ... the command in full is RESTORE
 LARNITE                 OLIVINE:I               PSEUDO_WOLLASTONITE
 QUARTZ                  RANKINITE  RESTORED
TDB_OXDEMO: rest ph tridymite wollastonite
   ... the command in full is RESTORE
 TRIDYMITE               WOLLASTONITE:I  RESTORED
TDB_OXDEMO: @@ To avoid complications we should also reject the Si+4 in the
TDB_OXDEMO: @@ first sublattice in the liquid phase. When there is oxygen present
TDB_OXDEMO: @@ all Si will form SiO2 or SiO4/-4. The Si+4 ion is needed only
TDB_OXDEMO: @@ for the liquid in systems without oxygen.
TDB_OXDEMO: rej const ionic_liq
   ... the command in full is REJECT
SUBLATTICE NUMBER: 1
CONSTITUENT: si+4
 SI+4 IN IONIC_LIQ:Y SUBLATTICE   1 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
 IONIC_LIQ:Y :CA+2:O-2 SIO4-4 SIO2:
  > Ionic liquid mixture, modelled by the ionic two-sublattice model.
 CRISTOBALITE :SIO2:
  > Prototype SiO2 (cF24, Fd3m)
 HALITE:I    :CA+2 VA:O-2:
  > This is CaO and FeO (cI2, Im-3m)
 HATRURITE   :CA+2:SI+4:O-2:
  > This is 3CaO.SiO2 (hR81, R3m)
 LARNITE     :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 (metastable at 1 atm)
 OLIVINE:I   :CA+2:CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 and fayalite
 PSEUDO_WOLLASTONITE :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (mS120, C12/c1)
 QUARTZ      :SIO2:
  > Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))
 RANKINITE   :CA+2:SI+4:O-2:
  > This is 3CaO.2SiO2 (mP48, P121/c1)
 TRIDYMITE   :SIO2:
  > Prototype SiO2 (hP12, P63/mmc)
 WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (aP30, P-1)
TDB_OXDEMO:Hit RETURN to continue
TDB_OXDEMO:
TDB_OXDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, Private Communication, liquid and solid Al2O3,CaO, MgO'
  'M. Hillert, B. Sundman and X. Wang, Calphad, 15 (1991), 53-58; CaO-SiO2'
  'T.I. Barry, NPL, UK, Unpublished research 1987; liquid and solid SiO2'
  'M. Hillert, B. Sundman and X. Wang, Metall Trans B, 21B (1990), 303-312;
      CaO-SiO2'
  'W. Huang, M. Hillert and X. Wang, Metall Mater Trans A, 26A (1995), 2293
      -2231; CaO-MgO-SiO2'
 -OK-
TDB_OXDEMO: @@ There is a miscibility gap in the ionic liquid close to SiO2.
TDB_OXDEMO: @@ In this database two composition sets will be created automatically
TDB_OXDEMO: @@ and one will have SiO2 as major constituent
TDB_OXDEMO:
TDB_OXDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3:
POLY_3: @@ Define more convenient components than the elements
POLY_3:
POLY_3: list-stat cps
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
```

```
 CA                        ENTERED   SER
 O                         ENTERED   SER
 SI                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                     STATUS    DRIVING FORCE   MOLES
 WOLLASTONITE              ENTERED      0.000000E+00    0.000000E+00
 TRIDYMITE                 ENTERED      0.000000E+00    0.000000E+00
 RANKINITE                 ENTERED      0.000000E+00    0.000000E+00
 QUARTZ                    ENTERED      0.000000E+00    0.000000E+00
 PSEUDO_WOLLASTONITE       ENTERED      0.000000E+00    0.000000E+00
 OLIVINE                   ENTERED      0.000000E+00    0.000000E+00
 LARNITE                   ENTERED      0.000000E+00    0.000000E+00
 HATRURITE                 ENTERED      0.000000E+00    0.000000E+00
 HALITE                    ENTERED      0.000000E+00    0.000000E+00
 CRISTOBALITE              ENTERED      0.000000E+00    0.000000E+00
 IONIC_LIQ#2               ENTERED      0.000000E+00    0.000000E+00
 IONIC_LIQ                 ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CA      ENTERED    O       ENTERED    O2SI2   ENTERED    SI3     ENTERED
 CA+2    ENTERED    O-2     ENTERED    O3      ENTERED    SIO2    ENTERED
 CA1O1   ENTERED    O1SI1   ENTERED    SI      ENTERED    SIO4-4  ENTERED
 CA2     ENTERED    O2      ENTERED    SI+4    ENTERED    VA      ENTERED
 CAO     ENTERED    O2-2    ENTERED    SI2     ENTERED    VA-2    ENTERED
 E-      ENTERED    O2SI1   ENTERED    SI2O7-6 ENTERED
POLY_3: def-com cao sio2 o
   ... the command in full is DEFINE_COMPONENTS
POLY_3: l-st cps
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                 STATUS    REF. STATE     T(K)           P(Pa)
 VA                        ENTERED   SER
 CAO                       ENTERED   SER
 SIO2                      ENTERED   SER
 O                         ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                     STATUS    DRIVING FORCE   MOLES
 WOLLASTONITE              ENTERED      0.000000E+00    0.000000E+00
 TRIDYMITE                 ENTERED      0.000000E+00    0.000000E+00
 RANKINITE                 ENTERED      0.000000E+00    0.000000E+00
 QUARTZ                    ENTERED      0.000000E+00    0.000000E+00
 PSEUDO_WOLLASTONITE       ENTERED      0.000000E+00    0.000000E+00
 OLIVINE                   ENTERED      0.000000E+00    0.000000E+00
 LARNITE                   ENTERED      0.000000E+00    0.000000E+00
 HATRURITE                 ENTERED      0.000000E+00    0.000000E+00
 HALITE                    ENTERED      0.000000E+00    0.000000E+00
 CRISTOBALITE              ENTERED      0.000000E+00    0.000000E+00
 IONIC_LIQ#2               ENTERED      0.000000E+00    0.000000E+00
 IONIC_LIQ                 ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CA      ENTERED    O       ENTERED    O2SI2   ENTERED    SI3     ENTERED
 CA+2    ENTERED    O-2     ENTERED    O3      ENTERED    SIO2    ENTERED
 CA1O1   ENTERED    O1SI1   ENTERED    SI      ENTERED    SIO4-4  ENTERED
 CA2     ENTERED    O2      ENTERED    SI+4    ENTERED    VA      ENTERED
 CAO     ENTERED    O2-2    ENTERED    SI2     ENTERED    VA-2    ENTERED
 E-      ENTERED    O2SI1   ENTERED    SI2O7-6 ENTERED
POLY_3:Hit RETURN to continue
POLY_3: s-c t=2000,p=1e5,n=1,w(sio2)=.9
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=2000, P=1E5, N=1, W(SIO2)=0.9
 DEGREES OF FREEDOM 1
POLY_3: @@ There is one degree of freedom due to the oxygen. As the oxygen content
POLY_3: @@ is determined by the Ca/Si ration there is no possibility to vary
POLY_3: @@ the oxygen content in this system independently. Thus the
POLY_3: @@ oxygen potential can be set to any value (larger than zero).
POLY_3: s-c ac(o)=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          2023 grid points in             0 s
    51 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: @@ Option N is used to include information on the
POLY_3: @@ constitution of the phases.
POLY_3: l-e screen
   ... the command in full is LIST_EQUILIBRIUM
Options /VWCS/: n
 Output from POLY-3, equilibrium =     1, label A0  , database: OXDEMO

 Conditions:
 T=2000, P=1E5, N=1, W(SIO2)=0.9, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature   2000.00 K (  1726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.96571E+01
 Total Gibbs energy -1.10541E+06,  Enthalpy -7.53274E+05,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 CAO                      1.0638E-01  1.0000E-01 6.4224E-25 -9.2632E+05 SER
 SIO2                     8.9362E-01  9.0000E-01 3.7467E-30 -1.1267E+06 SER
 O                        0.0000E+00  3.6248E-18 1.0000E+00  0.0000E+00 SER

 IONIC_LIQ#2                  Status ENTERED     Driving force  0.0000E+00
 Moles 6.7245E-01, Mass 4.0314E+01, Volume fraction 0.0000E+00  Mass fractions:
 SIO2  9.69163E-01  CAO   3.08366E-02  O     0.00000E+00
 Constitution:
 Sublattice  1,  Number of sites  6.8156E-02
 CA+2    1.00000E+00
 Sublattice  2,  Number of sites  2.0000E+00
 SIO2    9.82793E-01  SIO4-4  1.68709E-02  O-2     3.36172E-04

 IONIC_LIQ                    Status ENTERED     Driving force  0.0000E+00
 Moles 3.2755E-01, Mass 1.9343E+01, Volume fraction 0.0000E+00  Mass fractions:
 SIO2  7.55851E-01  CAO   2.44149E-01  O     0.00000E+00
 Constitution:
 Sublattice  1,  Number of sites  6.9176E-01
 CA+2    1.00000E+00
 Sublattice  2,  Number of sites  2.0000E+00
 SIO2    8.26780E-01  SIO4-4  1.72662E-01  O-2     5.57209E-04
POLY_3:Hit RETURN to continue
POLY_3: @@ The result shows the expected miscibility gap. However, in some
POLY_3: @@ cases the first calculation may fail. In such cases try to simplify the
```

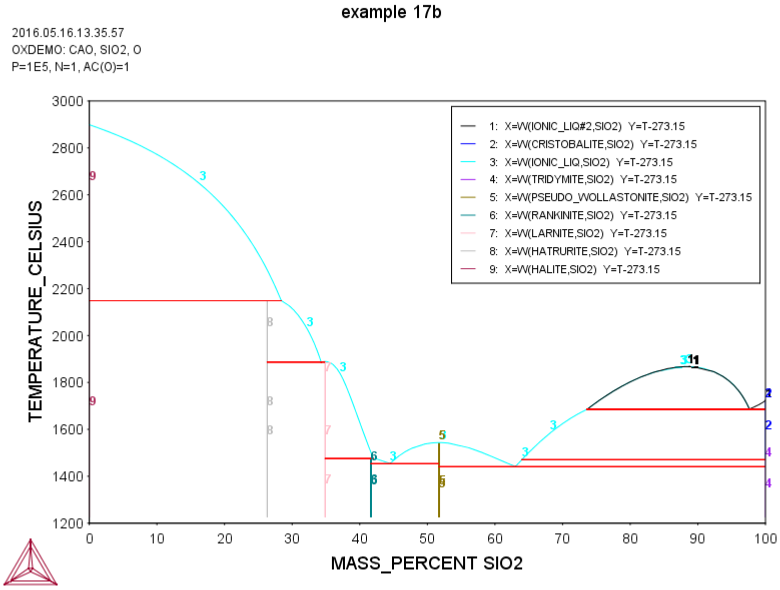
```
POLY_3: @@ calculation by suspending all phases but the important ones.
POLY_3: @@ Save the results so far on file
POLY_3:
POLY_3: save tcex17 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ Set the axis
POLY_3: s-a-v 1 w(sio2)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1500
Max value /1/: 3500
Increment /50/: 20
POLY_3: save tcex17 Y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16

 Phase region boundary   1 at:   9.053E-01  1.959E+03
     IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE
 Calculated                      19  equilibria

 Phase region boundary   2 at:   9.053E-01  1.959E+03
     IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE
 Calculated                      16  equilibria

 Phase region boundary   3 at:   9.053E-01  1.959E+03
     IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE
 Calculated                      19  equilibria

 Phase region boundary   4 at:   9.053E-01  1.959E+03
     IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE
 Calculated                      16  equilibria

 Phase region boundary   5 at:   9.053E-01  1.959E+03
     IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE
 Calculated                      19  equilibria

 Phase region boundary   6 at:   9.053E-01  1.959E+03
     IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE
 Calculated                      16  equilibria

 Phase region boundary   7 at:   9.053E-01  1.959E+03
     IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE
 Calculated                      19  equilibria

 Phase region boundary   8 at:   9.053E-01  1.959E+03
     IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE
 Calculated                      16  equilibria

 Phase region boundary   9 at:   8.835E-01  2.137E+03
  ** IONIC_LIQ
     IONIC_LIQ#2
 Calculated.                      10  equilibria

 Phase region boundary  10 at:   8.348E-01  1.959E+03
  ** IONIC_LIQ
     IONIC_LIQ#2
  ** CRISTOBALITE

 Phase region boundary  11 at:   9.882E-01  1.959E+03
```

```
    IONIC_LIQ#2
 ** CRISTOBALITE
Calculated                     18  equilibria

Phase region boundary  12 at:   8.695E-01  1.959E+03
    IONIC_LIQ
 ** CRISTOBALITE
Calculated.                     12  equilibria

Phase region boundary  13 at:   8.222E-01  1.744E+03
    IONIC_LIQ
 ** CRISTOBALITE
 ** TRIDYMITE

Phase region boundary  14 at:   8.222E-01  1.744E+03
    IONIC_LIQ
 ** TRIDYMITE
Calculated.                      3  equilibria

Phase region boundary  15 at:   8.175E-01  1.714E+03
    IONIC_LIQ
 ** PSEUDO_WOLLASTONITE
 ** TRIDYMITE

Phase region boundary  16 at:   5.740E-01  1.714E+03
    IONIC_LIQ
 ** PSEUDO_WOLLASTONITE
Calculated.                     22  equilibria

Phase region boundary  17 at:   4.813E-01  1.727E+03
    IONIC_LIQ
 ** PSEUDO_WOLLASTONITE
 ** RANKINITE

Phase region boundary  18 at:   4.309E-01  1.727E+03
    IONIC_LIQ
 ** RANKINITE
Calculated.                      3  equilibria

Phase region boundary  19 at:   4.184E-01  1.749E+03
    IONIC_LIQ
 ** LARNITE
 ** RANKINITE

Phase region boundary  20 at:   3.845E-01  1.749E+03
    IONIC_LIQ
 ** LARNITE
Calculated.                     39  equilibria

Phase region boundary  21 at:   3.459E-01  2.160E+03
    IONIC_LIQ
 ** HATRURITE
 ** LARNITE

Phase region boundary  22 at:   3.032E-01  2.160E+03
    IONIC_LIQ
 ** HATRURITE
Calculated.                     16  equilibria

Phase region boundary  23 at:   2.736E-01  2.422E+03
    IONIC_LIQ
 ** HALITE
 ** HATRURITE

Phase region boundary  24 at:   1.433E-01  2.422E+03
    IONIC_LIQ
 ** HALITE
Calculated                     53  equilibria

Phase region boundary  25 at:   1.327E-01  2.422E+03
 ** HALITE
    HATRURITE
Calculated..                     48  equilibria
Terminating at axis limit.

Phase region boundary  26 at:   3.061E-01  2.160E+03
 ** HATRURITE
    LARNITE
Calculated..                     34  equilibria
Terminating at axis limit.

Phase region boundary  27 at:   3.828E-01  1.749E+03
 ** LARNITE
    RANKINITE
Calculated..                     14  equilibria
Terminating at axis limit.

Phase region boundary  28 at:   4.671E-01  1.727E+03
    PSEUDO_WOLLASTONITE
 ** RANKINITE
Calculated..                     13  equilibria
Terminating at axis limit.

Phase region boundary  29 at:   7.627E-01  1.714E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated..                     12  equilibria
Terminating at axis limit.

Phase region boundary  30 at:   1.000E+00  1.744E+03
    CRISTOBALITE
 ** TRIDYMITE

Phase region boundary  31 at:   8.574E-01  1.959E+03
 ** IONIC_LIQ
    IONIC_LIQ#2
Calculated.                     35  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   8.835E-01  2.137E+03
 ** IONIC_LIQ
    IONIC_LIQ#2
Calculated                      6  equilibria

Phase region boundary  33 at:   8.835E-01  2.137E+03
 ** IONIC_LIQ
```

```
    IONIC_LIQ#2
Calculated.                      10  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:    8.835E-01  2.137E+03
 ** IONIC_LIQ
    IONIC_LIQ#2
Calculated                       7  equilibria

Phase region boundary  35 at:    8.835E-01  2.137E+03
 ** IONIC_LIQ
    IONIC_LIQ#2
Calculated.                      10  equilibria
Terminating at known equilibrium

Phase region boundary  36 at:    8.835E-01  2.137E+03
 ** IONIC_LIQ
    IONIC_LIQ#2
Calculated.                      25  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:    8.835E-01  2.137E+03
 ** IONIC_LIQ
    IONIC_LIQ#2
Calculated.                      10  equilibria
Terminating at known equilibrium

Phase region boundary  38 at:    8.835E-01  2.137E+03
 ** IONIC_LIQ
    IONIC_LIQ#2
Calculated                       6  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex17\tcex
17.POLY3
CPU time for mapping                       2  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x w-p sio2
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 17a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Indentify the phases with labels
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: f
POST:
POST: set-title example 17b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex18

```
About Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex18\tcex18.TCM" set-echo
SYS: @@
SYS: @@ Calculation
SYS: @@ of the A3 temperature
SYS: @@ of a steel and the influence
SYS: @@ of each alloying element on
SYS: @@ this temperature
SYS: @@
SYS: @@
SYS: @@ A3 temperature is the temperature where ferrite starts to form from
SYS: @@ austenite. One can easily read A3 from Fe-C phase diagram. But for
SYS: @@ complex multicomponent steels, no simple diagram can be used.
SYS: @@ This example shows how to calculate the A3 temperature of a steel.
SYS: @@ Using the facility in POLY, it is easy to find out the influence
SYS: @@ of each alloying element on A3 temperature. This information is
SYS: @@ useful if one wants to modify the compositions of a steel but keep
SYS: @@ A3 unchanged.
SYS: @@
SYS: set-log ex18,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: cr 1.5 mn .5 c .3 si .3 nb .1
Next alloying element:
Temperature (C) /1000/: 1100
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NB  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M6C                      M5C2
 M3C2                     KSI_CARBIDE              A1_KAPPA
 KAPPA                    Z_PHASE                  FE4N_LP1
 FECN_CHI                 SIGMA                    MU_PHASE
 CHI_A12                  LAVES_PHASE_C14          M3SI
 G_PHASE                  CR3SI                    FE2SI
 MSI                      M5SI3                    NBNI3
 AL4C3                    FE8SI2C                  SIC

Reject phase(s) /NONE/: ?

 Reject phase(s)

  This is a question generated by the database allowing the user to select
  the phases. Normally, all phases should be included and the user just
  presses <RETURN>.

  If a phase is to be rejected, the name of the phase must be supplied.
  Several phase names can be specified in one line.

  It is possible to reject all phase by giving an asterisk "*". If the
  number of phases to be included is much smaller than the total number
  of phases, it may be convenient to first reject all phases and then
  restore just those that should be included.

  Note: This question will be repeated until the user press <RETURN>
        after rejected all undesired phases or an asterisk "*".


Reject phase(s) /NONE/: *
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M6C                     M5C2
 M3C2                    KSI_CARBIDE             A1_KAPPA
 KAPPA                   Z_PHASE                 FE4N_LP1
 FECN_CHI                SIGMA                   MU_PHASE
 CHI_A12                 LAVES_PHASE_C14         M3SI
 G_PHASE                 CR3SI                   FE2SI
 MSI                     M5SI3                   NBNI3
```

```
 AL4C3                   FE8SI2C                 SIC
   REJECTED
Restore phase(s):: liq fcc_a1 bcc_a2 hcp_a3 graphite cementite m23 m7
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  GRAPHITE                CEMENTITE
 M23C6                   M7C3  RESTORED
Restore phase(s): /NONE/:

 .......................................................

    The following phases are retained in this system:

 LIQUID:L                 BCC_A2                   FCC_A1
 HCP_A3                   GRAPHITE                 CEMENTITE
 M23C6                    M7C3

 .......................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

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  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
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  'B.-J. Lee, Metall. Mater. Trans. A, 32A, 2423-39(2001); Fe-Nb'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         10008 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3:
POLY_3:
POLY_3: @@ In the TCFE database the number of phases is very large.
POLY_3: @@ It is strongly recommended that one rejects all phases
POLY_3: @@ that one knows should not be stable
POLY_3:
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
    P=1E5, N=1
 DEGREES OF FREEDOM 0
```

```
 Temperature   1373.15 K (  1100.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50375E+01
 Total Gibbs energy -7.21999E+04,  Enthalpy  4.05686E+04,  Volume  7.32058E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3747E-02  3.0000E-03 1.0740E-02 -5.1763E+04 SER
 CR                      1.5877E-02  1.5000E-02 1.3123E-04 -1.0205E+05 SER
 FE                      9.5890E-01  9.7300E-01 2.0390E-03 -7.0732E+04 SER
 MN                      5.0091E-03  5.0000E-03 4.2846E-06 -1.4112E+05 SER
 NB                      5.9240E-04  1.0000E-03 1.3310E-07 -1.8076E+05 SER
 SI                      5.8788E-03  3.0000E-03 1.1131E-08 -2.0909E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.9900E-01, Mass 5.4984E+01, Volume fraction 9.9904E-01  Mass fractions:
 FE  9.73932E-01  MN  5.00479E-03  C   2.89608E-03
 CR  1.50122E-02  SI  3.00290E-03  NB  1.51584E-04

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0011E-03, Mass 5.3091E-02, Volume fraction 9.5720E-04  Mass fractions:
 NB  8.79676E-01  FE  7.33072E-03  MN  3.71964E-05
 C   1.10624E-01  CR  2.33143E-03  SI  1.24275E-09
POLY_3:Hit RETURN to continue
POLY_3: @@ Two FCC phases are stable, one with mainly Fe and
POLY_3: @@ one with mainly Nb and C, which is the NbC carbide.
POLY_3: @@ The second fcc is called FCC#2. The digit after # is
POLY_3: @@ called composition set but can be ignored if it is unity.
POLY_3:
POLY_3: li-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 NB                      ENTERED   SER
 SI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FCC_A1#2                ENTERED      0.000000E+00    1.001053E-03
 FCC_A1                  ENTERED      0.000000E+00    9.989989E-01
 BCC_A2                  ENTERED     -1.877374E-02    0.000000E+00
 LIQUID                  ENTERED     -2.093926E-01    0.000000E+00
 HCP_A3                  ENTERED     -3.238293E-01    0.000000E+00
 HCP_A3#2                ENTERED     -3.238293E-01    0.000000E+00
 M23C6                   ENTERED     -3.975771E-01    0.000000E+00
 CEMENTITE               ENTERED     -4.579912E-01    0.000000E+00
 M7C3                    ENTERED     -6.050859E-01    0.000000E+00
 GRAPHITE                ENTERED     -2.504689E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 C   ENTERED    C4  ENTERED    CR  ENTERED    NB  ENTERED
 C2  ENTERED    C5  ENTERED    FE  ENTERED    SI  ENTERED
 C3  ENTERED    C60 ENTERED    MN  ENTERED    VA  ENTERED
POLY_3:
POLY_3: @@ Fcc appears twice on the list above. The HCP phase also has
POLY_3: @@ two composition sets.
POLY_3:
POLY_3: @@ This result looks reasonable, save it on a file
POLY_3: save tcex18 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: @@ Now calculate when bcc (ferrite) begins to form
POLY_3: @@ using the COMPUTE-TRANSITION command
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
 You must release one of these conditions
 T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
 P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
 Testing POLY result by global minimization procedure
Calculated         10008 grid points in             1 s
To form BCC_A2 the condition is set to T=1071.60881565
POLY_3:Hit RETURN to continue
POLY_3: @@ We may expect BCC to form at a lower temperature, because sometimes
POLY_3: @@ a higer temperature is found as there is a delta-ferrite stable
POLY_3: @@ at high temperatures.
POLY_3: @@
POLY_3: @@ Calculate again the equilibrium at lower temperature.  You can
POLY_3: @@ do this by just a SET-COND T=... command but then the temperature must
POLY_3: @@ be given in Kelvin.  You can use the DEF-MAT command to do this
POLY_3: @@ in Celsius
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
Same elements as before? /Y/: Y
Mass (weight) percent of C /.3/: .3
Mass (weight) percent of CR /1.5/: 1.5
Mass (weight) percent of MN /.5/: .5
Mass (weight) percent of NB /.1/: .1
Mass (weight) percent of SI /.3/: .3
Temperature (C) /798/: 800
 Using global minimization procedure
Calculated         10008 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
    P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1073.15 K (   800.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50375E+01
 Total Gibbs energy -4.87895E+04,  Enthalpy  3.03117E+04,  Volume  7.17692E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
```

```
 C                        1.3747E-02  3.0000E-03 4.4068E-02 -2.7857E+04 SER
 CR                       1.5877E-02  1.5000E-02 3.5554E-04 -7.0863E+04 SER
 FE                       9.5890E-01  9.7300E-01 4.8677E-03 -4.7515E+04 SER
 MN                       5.0091E-03  5.0000E-03 8.2064E-06 -1.0449E+05 SER
 NB                       5.9240E-04  1.0000E-03 2.9934E-09 -1.7512E+05 SER
 SI                       5.8788E-03  3.0000E-03 8.9756E-10 -1.8587E+05 SER

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.9870E-01, Mass 5.4971E+01, Volume fraction 9.9878E-01  Mass fractions:
 FE  9.74156E-01  MN  5.00593E-03  C   2.86369E-03
 CR  1.49685E-02  SI  3.00361E-03  NB  2.74704E-06

 FCC_A1#2                     Status ENTERED     Driving force  0.0000E+00
 Moles 1.2984E-03, Mass 6.6134E-02, Volume fraction 1.2211E-03  Mass fractions:
 NB  8.29930E-01  CR  4.11711E-02  MN  7.37925E-05
 C   1.16301E-01  FE  1.25236E-02  SI  1.74994E-10
POLY_3:
POLY_3: @@ Try a slightly different COMPUTE-TRANSITION command.
POLY_3: @@ This finds the first phase change in the specified direction.
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: any
 You must release one of these conditions
 T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
 P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Estimated change (with sign) /1/: ?

 Estimated change (with sign)

  A given varying direction sign and an estimated change of the released
  condition, in this case X(FE), must be given here: a negative sign means
  at a lower value of the released condition any new phase is to be found,
  and a positive sign at a higher value; an estimated change of the released
  condition implies where any new phase is expected (but it is only estimated
  value, so any value within its reasonable scale would be enough).

  For instance, if a combination of -.02 is input, the following message may
  come up (after a successful calculation):
    To form BCC_A2#1 the condition is set to X(FE)=.493708756187

  This calculated value will then be assign as the parameter of that removed
  condition, in this case, the X(FE) variable. So the following message will
  be shown on the screen, if the LIST_CONDITIONS command is typed:
    P=100000, T=800, N=1, X(FE)=4.93708756E-1
    DEGREES OF FREEDOM 0


Estimated change (with sign) /1/: -1
 Testing POLY result by global minimization procedure
Calculated         10008 grid points in              0 s
To form BCC_A2#1 the condition is set to T=1071.60881565
POLY_3: show t
   ... the command in full is SHOW_VALUE
 T=1071.6088
POLY_3: @@ The transition temperature to form BCC is the same.
POLY_3: @@ If we want it in Celsius enter a function for that.
POLY_3: enter fun tc=t-273;
   ... the command in full is ENTER_SYMBOL
POLY_3: show tc
   ... the command in full is SHOW_VALUE
 TC=798.60882
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ This is the minimum temperature for hardening because below this
POLY_3: @@ temperature ferrite will form from austenite. Check how a small
POLY_3: @@ change of the composition can change this temperature. We must
POLY_3: @@ then set bcc as fix and release the condition on the temperature.
POLY_3: c-st p bcc_a2=fix 0
   ... the command in full is CHANGE_STATUS
POLY_3: s-c t=none
   ... the command in full is SET_CONDITION
POLY_3: @@ The change of the calculated temperature for a small change of
POLY_3: @@ the amount of a component can be calculated as a derivative
POLY_3: @@ using the dot "." between the calculated variable and the condition.
POLY_3: sh t.w(mn)
   ... the command in full is SHOW_VALUE
 T.W(MN)=-2592.1917
POLY_3: sh t.w(cr)
   ... the command in full is SHOW_VALUE
 T.W(CR)=-781.45507
POLY_3: sh t.w(nb)
   ... the command in full is SHOW_VALUE
 T.W(NB)=3005.9537
POLY_3: sh t.w(c)
   ... the command in full is SHOW_VALUE
 T.W(C)=-21796.295
POLY_3: sh t.w(si)
   ... the command in full is SHOW_VALUE
 T.W(SI)=2990.1116
POLY_3:Hit RETURN to continue
POLY_3: @@ A negative value means the temperature will decrease if the
POLY_3: @@ amount is increased. Check for Mn
POLY_3: s-c w(mn)
   ... the command in full is SET_CONDITION
Value /.005/: .01
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         10008 grid points in              0 s
     9 ITS,  CPU TIME USED   0 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1058.9661
POLY_3:Hit RETURN to continue
POLY_3: @@ The temperature decreased from 1072 to 1059 i.e. 13 degrees.
POLY_3: @@ According to the derivatives calculated above, one could increase
POLY_3: @@ the temperature with the same amount by increasing the amount of Si
POLY_3: @@ 2592/2990=0.8669 times of the change in Mn i.e. from 0.3 to 0.733 %
POLY_3: s-c w(si)
   ... the command in full is SET_CONDITION
```

```
Value /.003/: .00733
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         10008 grid points in             0 s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1070.73
POLY_3: @@ The facility to calculate these derivatives is a powerful feature
POLY_3: @@ in order to find the best way to obtain a certain property of a material.
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3:
```

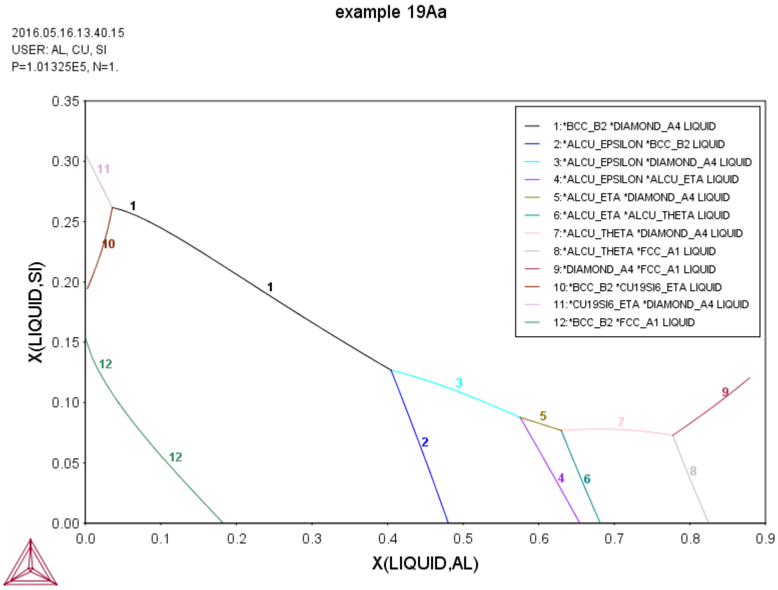
tcex19A

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tcex19A.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS: @@    Part A: step-by-step calculation
SYS: @@
SYS: set-log ex19a,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw USER tcex19_cost2
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
TDB_USER: d-sys
   ... the command in full is DEFINE_SYSTEM
ELEMENTS: cu al si
 CU                      AL                      SI
   DEFINED
TDB_USER: l-s c
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :AL CU SI:
 ALCE_AMORPHOUS :AL:
 ALCUZN_T    :AL:CU VA:
 ALCU_DELTA  :AL:CU:
 ALCU_EPSILON :AL CU:CU:
 ALCU_ETA    :AL CU:CU:
 ALCU_PRIME  :AL:CU:
 ALCU_THETA  :AL:AL CU:
 ALCU_ZETA   :AL:CU:
 ALLI        :AL:VA:
 ALMO        :AL:AL:
 ALM_D019    :AL:AL:
 ALND_AMORPHOUS :AL:
 ALTI        :AL:AL:
 BCC_A2      :AL CU SI:VA:
 BCC_B2      :AL CU SI:AL CU SI:VA:
 BCT_A5      :AL:
 CBCC_A12    :AL SI:VA:
 CR3SI_A15   :SI:AL SI:
 CRSI2       :SI:SI:
 CU19SI6_ETA :CU:SI:
 CU33SI7_DELTA :CU:SI:
 CU4SI_EPSILON :CU:SI:
 CU56SI11_GAMMA :CU:SI:
 CU6Y        :CU:CU2:
 CUB_A13     :AL SI:VA:
 CUB_A15     :SI:AL SI:
 DIAMOND_A4  :AL SI:
 FCC_A1      :AL CU SI:VA:
 GAMMA_D83   :AL:AL CU:CU:
 GAMMA_H     :AL:AL CU:CU:
 HCP_A3      :AL CU SI:VA:
 HCP_ZN      :AL CU SI:VA:
 LAVES_C14   :AL CU:AL CU:
 LAVES_C15   :AL CU SI:AL CU SI:
 LAVES_C36   :AL CU:AL CU:
 SIV3        :SI:SI:
TDB_USER: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 Reference REF1       missing close to line                    641
 Reference REF1       missing close to line                    643
 Reference REF1       missing close to line                    645
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1300,p=101325,n=1
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1300, P=1.01325E5, N=1
 DEGREES OF FREEDOM 2
POLY_3: s-c x(si)=.25,x(al)=.2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16220 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: vwcs
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
```

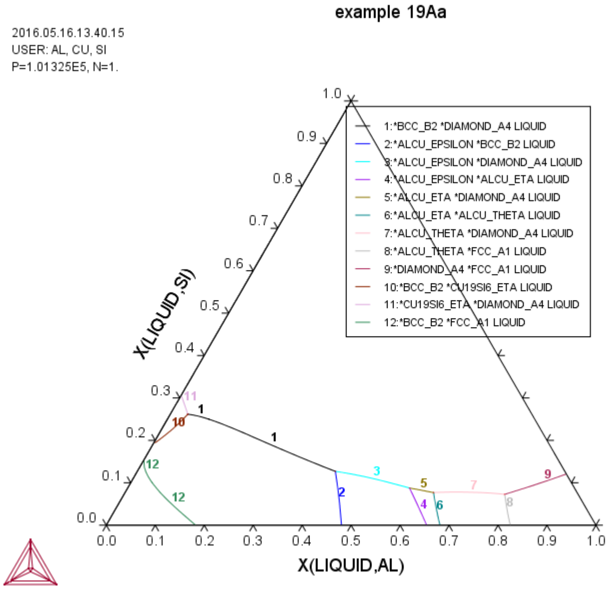
```
 T=1300, P=1.01325E5, N=1, X(SI)=0.25, X(AL)=0.2
 DEGREES OF FREEDOM 0

 Temperature   1300.00 K (  1026.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.73679E+01
 Total Gibbs energy -8.02595E+04,  Enthalpy  3.22931E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                       2.0000E-01  1.1393E-01 5.1836E-05 -1.0666E+05 SER
 CU                       5.5000E-01  7.3785E-01 4.1349E-04 -8.4211E+04 SER
 SI                       2.5000E-01  1.4823E-01 9.3957E-03 -5.0450E+04 SER

 LIQUID                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.7368E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  7.37847E-01  SI  1.48228E-01  AL  1.13925E-01
POLY_3:Hit RETURN to continue
POLY_3: @@ we want to calculate the monovariant lines with liquid. Select
POLY_3: @@ two compositions and the temperature as axis
POLY_3: s-a-v 1 x(al)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .01
POLY_3: s-a-v 2 x(si)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .01
POLY_3: s-a-v 3 t 500 2000 25
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: @@Set liquid as "present", otherwise all monovariant lines will be calculated.
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: ?
 EQUILIBRIUM_CALCUL        NEW_COMPOSITION_SET       SHOW_FOR_T=
 GLOBAL_MINIMIZATION       OUTPUT_FILE_FOR_SHOW      STABILITY_CHECK
 IGNORE_COMPOSI_SET_ORDER PARAEQUILIBRIUM           STEP_AND_MAP
 LIST_PHASE_ADDITION       PHASE_ADDITION            T-ZERO TEMPERATURE
 MAJOR_CONSTITUENTS        PRESENT_PHASE             TOGGLE_ALTERNATE_MODE
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liquid
POLY_3:
POLY_3: save tcex19a1 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point    1
 Generating start point    2

 Phase region boundary   1 at:   8.426E-02  2.500E-01  1.182E+03
     LIQUID
  ** BCC_B2
  ** DIAMOND_A4
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tce
 x19a1.POLY3
 CALCULATED    35 EQUILIBRIA

 Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
     LIQUID
     ALCU_EPSILON
  ** BCC_B2
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
     LIQUID
  ** ALCU_EPSILON
  ** BCC_B2
 Terminating at diagram limit
 CALCULATED    18 EQUILIBRIA

 Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4
 CALCULATED    20 EQUILIBRIA

 Phase region boundary   2 at:   5.755E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_EPSILON
     ALCU_ETA
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   5.755E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA
 Terminating at diagram limit
 CALCULATED    16 EQUILIBRIA

 Phase region boundary   2 at:   5.755E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_ETA
  ** DIAMOND_A4
 CALCULATED     8 EQUILIBRIA

 Phase region boundary   2 at:   6.299E-01  7.685E-02  8.291E+02
     LIQUID
  ** ALCU_ETA
     ALCU_THETA
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   6.299E-01  7.685E-02  8.291E+02
     LIQUID
  ** ALCU_ETA
  ** ALCU_THETA
 Terminating at diagram limit
 CALCULATED    13 EQUILIBRIA
```

```
 Phase region boundary   2 at:   6.299E-01  7.685E-02  8.291E+02
     LIQUID
  ** ALCU_THETA
  ** DIAMOND_A4
 CALCULATED    18 EQUILIBRIA

 Phase region boundary   2 at:   7.774E-01  7.282E-02  7.852E+02
     LIQUID
  ** ALCU_THETA
  ** DIAMOND_A4
     FCC_A1
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   7.774E-01  7.282E-02  7.852E+02
     LIQUID
  ** ALCU_THETA
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED    12 EQUILIBRIA

 Phase region boundary   2 at:   7.774E-01  7.282E-02  7.852E+02
     LIQUID
  ** DIAMOND_A4
  ** FCC_A1
 *** SORRY CANNOT CONTINUE ***    4

 CALCULATED    18 EQUILIBRIA

 Phase region boundary   2 at:   8.426E-02  2.500E-01  1.182E+03
     LIQUID
  ** BCC_B2
  ** DIAMOND_A4
 CALCULATED     8 EQUILIBRIA

 Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
     LIQUID
  ** BCC_B2
     CU19SI6_ETA
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
     LIQUID
  ** BCC_B2
  ** CU19SI6_ETA
 Terminating at diagram limit
 CALCULATED    12 EQUILIBRIA

 Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
     LIQUID
  ** CU19SI6_ETA
  ** DIAMOND_A4
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tce
 x19a1.POLY3
 CPU time for mapping                     1  seconds
POLY_3:
POLY_3: @@ The monovariant line FCC/BCC/LIQ in the Cu corner is not connected,
POLY_3: @@ so add a start point for that. This is different from a MAP with
POLY_3: @@ two axes, where all connected or non-connected lines can be found
POLY_3: @@ automatically.
POLY_3: read tcex19a1
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c x(al)=.1 x(si)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16220 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3:
POLY_3: map
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.390E-02  1.000E-01  1.285E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED    18 EQUILIBRIA

 Phase region boundary   2 at:   4.390E-02  1.000E-01  1.285E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tce
 x19a1.POLY3
 CPU time for mapping                     0  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: @@ we want the liquid compositions only
POST: s-d-a x x(liquid,al)
```

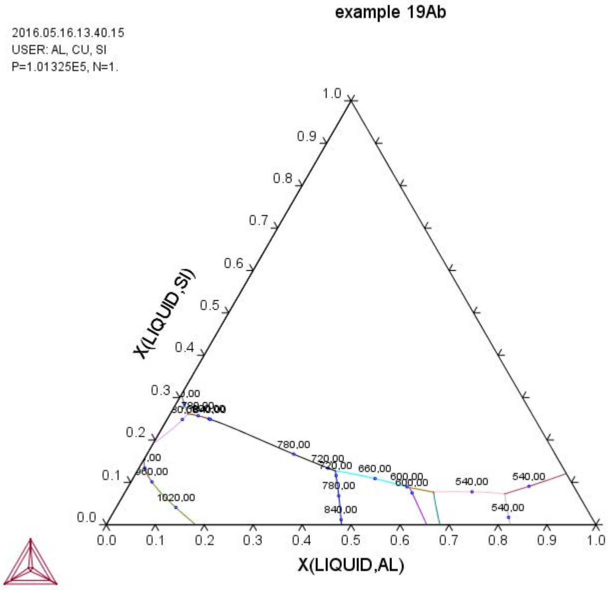
```
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liquid,si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 19Aa
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Make it triangular and scale the axis
POST: s-d-t
   ... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM  (Y OR N) /N/: y,,,,,,,
POST: s-sc y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-sc x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: @@ Plot the phases stable along the lines
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Take away the phase labels and add
POST: @@ tic marks along the lines (the Z axis)
POST: s-lab n
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a z t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-sc z n 500 1000
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 19Ab
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

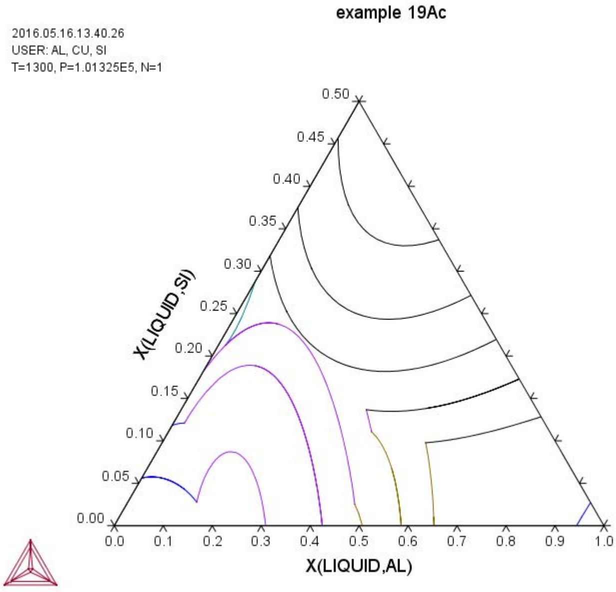


```
POST:
POST:Hit RETURN to continue
POST: @@ We will make a new calculation to overlay these monovariant lines
POST: @@ with isothermal calculations
POST:
POST: make tcex19a y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY_3: read tcex19a1
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-a-v 3
   ... the command in full is SET_AXIS_VARIABLE
Condition /T/: none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16220 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex19a2 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1300, P=1.01325E5, N=1, X(SI)=0.25, X(AL)=0.2
 DEGREES OF FREEDOM 0
POLY_3: s-c x(al)
   ... the command in full is SET_CONDITION
Value /.2/: .10
POLY_3: @@ One must use ADD to have several start points at different temperatures.
POLY_3: @@ But do not use default direction as that will create a lot of start points.
POLY_3: @@ Increasing the Si content will most certainly make a solid phase stable.
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: @@ One may have initial equilibria for several different
POLY_3: @@ conditions at the same time. Just the axis variables have
POLY_3: @@ to be the same
POLY_3: @@ To make nice isothermal curves is not easy, one has to try
POLY_3: @@ with several start points to find all curve sections.
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /1300/: 1200
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16220 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /1200/: 1100
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16220 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 2
```

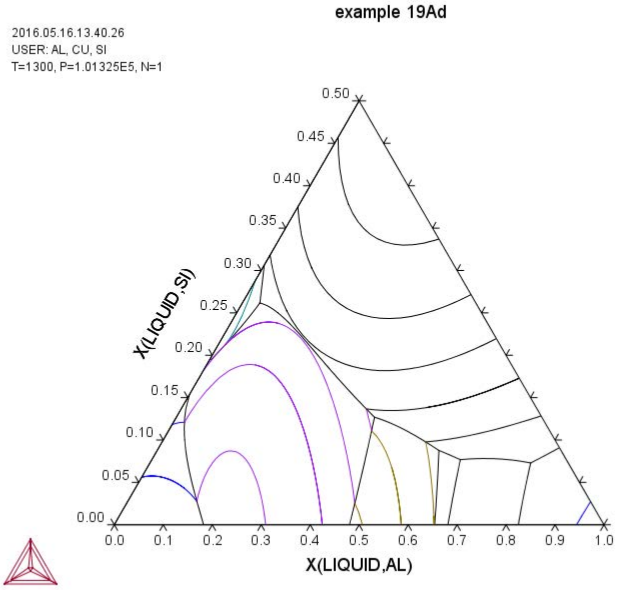
```
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: @@ This line exists only in Al rich corner
POLY_3: s-c x(al)=.5 x(si)=.1
   ... the command in full is SET_CONDITION
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /1100/: 1000
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16220 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: @@ A start point in the low melting Al corner too
POLY_3: s-c x(al)=.9 x(si)=.01 t=900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16220 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard

 Phase region boundary   1 at:   5.000E-02  6.891E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     10  equilibria

 Phase region boundary   2 at:   5.000E-02  6.891E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     52  equilibria

 Phase region boundary   3 at:   1.004E-01  3.055E-02
     LIQUID
  ** FCC_A1
 Calculated                     21  equilibria

 Phase region boundary   4 at:   1.004E-01  3.055E-02
     LIQUID
  ** FCC_A1
 Calculated.                      5  equilibria

 Phase region boundary   5 at:   1.373E-01  1.932E-02
     LIQUID
  ** BCC_B2
  ** FCC_A1

 Phase region boundary   6 at:   1.463E-01  2.848E-02
     LIQUID
  ** BCC_B2
 Calculated                     51  equilibria

 Phase region boundary   7 at:   1.373E-01  1.932E-02
     LIQUID
  ** FCC_A1
 Calculated                     27  equilibria

 Phase region boundary   8 at:   5.000E-02  6.515E-01
     LIQUID
  ** DIAMOND_A4
```

```
Calculated                     43  equilibria

Phase region boundary   9 at:   5.000E-02  6.515E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     52  equilibria

Phase region boundary  10 at:   1.081E-01  1.639E-01
    LIQUID
 ** BCC_B2
Calculated.                     16  equilibria

Phase region boundary  11 at:   2.872E-02  1.169E-01
    LIQUID
 ** BCC_B2
 ** FCC_A1

Phase region boundary  12 at:   2.764E-02  9.624E-02
    LIQUID
 ** FCC_A1
Calculated                     13  equilibria

Phase region boundary  13 at:   2.872E-02  1.169E-01
    LIQUID
 ** BCC_B2
Calculated                     70  equilibria

Phase region boundary  14 at:   1.081E-01  1.639E-01
    LIQUID
 ** BCC_B2
Calculated                     44  equilibria

Phase region boundary  15 at:   5.000E-02  6.262E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     38  equilibria

Phase region boundary  16 at:   5.000E-02  6.262E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     56  equilibria

Phase region boundary  17 at:   1.116E-01  1.999E-01
    LIQUID
 ** BCC_B2
Calculated                     23  equilibria

Phase region boundary  18 at:   1.116E-01  1.999E-01
    LIQUID
 ** BCC_B2
Calculated.                     34  equilibria

Phase region boundary  19 at:   4.370E-01  1.765E-02
    LIQUID
 ** ALCU_EPSILON
 ** BCC_B2

Phase region boundary  20 at:   4.453E-01  1.265E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                     18  equilibria

Phase region boundary  21 at:   4.370E-01  1.765E-02
    LIQUID
 ** BCC_B2
Calculated.                     43  equilibria

Phase region boundary  22 at:   2.106E-02  1.939E-01
    LIQUID
 ** BCC_B2
 ** CU19SI6_ETA

Phase region boundary  23 at:   7.190E-03  2.263E-01
    LIQUID
 ** CU19SI6_ETA
Calculated                     24  equilibria

Phase region boundary  24 at:   2.500E-01  5.691E-01
    LIQUID
 ** DIAMOND_A4
Calculated.                      8  equilibria

Phase region boundary  25 at:   1.890E-01  5.683E-01
    LIQUID
 ** BCC_B2
 ** DIAMOND_A4

Phase region boundary  26 at:   3.667E-01  1.003E-01
    LIQUID
 ** BCC_B2
Calculated.                      5  equilibria

Phase region boundary  27 at:   3.979E-01  7.953E-02
    LIQUID
 ** ALCU_EPSILON
 ** BCC_B2

Phase region boundary  28 at:   4.219E-01  5.542E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                     28  equilibria

Phase region boundary  29 at:   1.890E-01  5.683E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     42  equilibria

Phase region boundary  30 at:   2.500E-01  5.691E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     49  equilibria

Phase region boundary  31 at:   4.698E-01  3.348E-02
    LIQUID
 ** ALCU_EPSILON
Calculated.                      6  equilibria
```

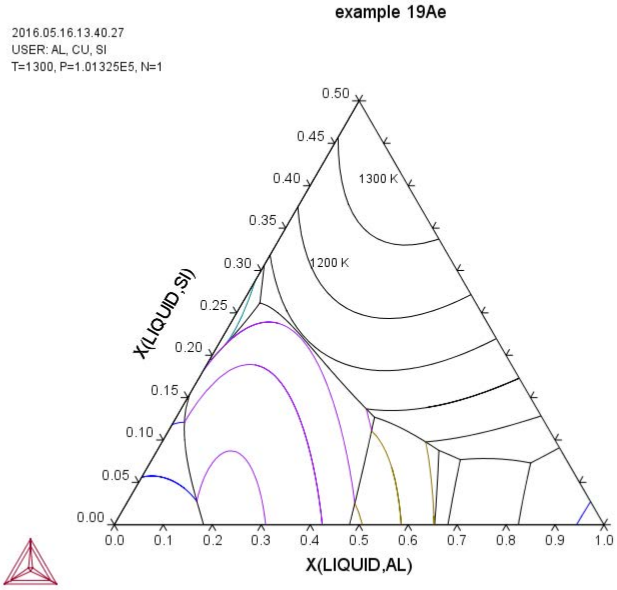
```
 Terminating at known equilibrium

 Phase region boundary  32 at:   4.698E-01  3.348E-02
     LIQUID
  ** ALCU_EPSILON
 Calculated                     27  equilibria

 Phase region boundary  33 at:   9.694E-01  5.516E-03
     LIQUID
  ** FCC_A1
 Calculated                     12  equilibria

 Phase region boundary  34 at:   9.694E-01  5.516E-03
     LIQUID
  ** FCC_A1
 Calculated                     16  equilibria

 Phase region boundary  35 at:   5.506E-01  5.000E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated                     18  equilibria

 Phase region boundary  36 at:   5.506E-01  5.000E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated.                     10  equilibria

 Phase region boundary  37 at:   4.954E-01  4.888E-02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4

 Phase region boundary  38 at:   2.690E-01  5.489E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     35  equilibria

 Phase region boundary  39 at:   4.954E-01  4.888E-02
     LIQUID
  ** ALCU_EPSILON
 Calculated                     22  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tce
 x19a2.POLY3
 CPU time for mapping                      7  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x x(liquid,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liquid,si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST:
POST:
POST: set-title example 19Ac
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex19a
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 19Ad
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: add .1 .4 n 1300 K
   ... the command in full is ADD_LABEL_TEXT
Text size: /.36/:
POST:
POST: add .1 .3 n 1200 K
   ... the command in full is ADD_LABEL_TEXT
Text size: /.36/:
POST:
POST: set-title example 19Ae
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex19B

```
AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\tcex19B.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS: @@    Part B: using TERNARY module
SYS: @@
SYS: @@ Using TERNARY module, one can easily obtain the information on
SYS: @@ invariant reactions, such as temperature and compositions.
SYS: @@
SYS: set-log ex19b,,
SYS: go ter
   ... the command in full is GOTO_MODULE

 Quick ternary phase diagram calculation module

 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 Current database: Iron Demo Database

 VA                      /-  DEFINED
Database: /FEDEMO/: user tcex19_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
First element: al cu si
Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/: L
Min temperature, C /25/: 25
Max temperature, C /2500/: 2500
Temperature interval /100/: 100
Global minimization on: /N/: N
 VA                      /-  DEFINED
 REINITIATING GES5 .....
 AL                      CU                      SI
   DEFINED
 *** GAS INPUT IGNORED

 **********************************************************
 * WARNING: This database has no list of assessed systems *
 *             The diagram may be wrong.                  *
 **********************************************************

Quit? /Y/: N
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 Reference REF1       missing close to line                    641
 Reference REF1       missing close to line                    643
 Reference REF1       missing close to line                    645
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
 -OK-
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 T = 1673.15 K
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   7.327E-03  9.853E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     15  equilibria

 Phase region boundary   2 at:   7.327E-03  9.853E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     15  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                       0  seconds
 T = 1573.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   7.453E-02  8.883E-01
     LIQUID
```

```
  ** DIAMOND_A4
 Calculated                     23  equilibria

 Phase region boundary   2 at:   7.453E-02  8.883E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     25  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                       0  seconds
 T = 1473.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   1.372E-01  7.942E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     30  equilibria

 Phase region boundary   2 at:   1.372E-01  7.942E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     22  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                       1  seconds
 T = 1373.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   1.926E-01  7.111E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     28  equilibria

 Phase region boundary   2 at:   1.926E-01  7.111E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     32  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                       0  seconds
 T = 1273.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   6.652E-01  9.329E-03
     LIQUID
  ** BCC_B2
 Calculated.                      2  equilibria

 Phase region boundary   2 at:   6.645E-01  6.795E-03
     LIQUID
  ** BCC_B2
  ** GAMMA_H

 Phase region boundary   3 at:   6.653E-01  4.077E-03
     LIQUID
  ** GAMMA_H
 Calculated                     12  equilibria

 Phase region boundary   4 at:   6.645E-01  6.795E-03
     LIQUID
  ** BCC_B2
 Calculated.                     29  equilibria

 Phase region boundary   5 at:   8.419E-01  6.666E-02
     LIQUID
  ** BCC_B2
  ** FCC_A1

 Phase region boundary   6 at:   8.633E-01  4.917E-02
     LIQUID
  ** FCC_A1
 Calculated                     25  equilibria

 Phase region boundary   7 at:   6.652E-01  9.329E-03
     LIQUID
  ** BCC_B2
 Calculated.                     30  equilibria
```

```
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      0  seconds

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   2.311E-01  6.535E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     34  equilibria

 Phase region boundary   2 at:   2.311E-01  6.535E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     34  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      0  seconds
 T = 1173.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   5.840E-01  7.591E-03
     LIQUID
  ** BCC_B2
 Calculated                      9  equilibria

 Phase region boundary   2 at:   5.840E-01  7.591E-03
     LIQUID
  ** BCC_B2
 Calculated.                     39  equilibria

 Phase region boundary   3 at:   8.543E-01  1.296E-01
     LIQUID
  ** BCC_B2
  ** FCC_A1

 Phase region boundary   4 at:   8.749E-01  1.099E-01
     LIQUID
  ** FCC_A1
 Calculated                     24  equilibria

 Phase region boundary   5 at:   8.543E-01  1.296E-01
     LIQUID
  ** BCC_B2
 Calculated                     54  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      1  seconds

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   2.562E-01  6.158E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     39  equilibria

 Phase region boundary   2 at:   2.562E-01  6.158E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     37  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      0  seconds
 T = 1073.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
```

```
 Phase region boundary   1 at:   5.198E-01  5.412E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated                     11  equilibria

 Phase region boundary   2 at:   5.198E-01  5.412E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated.                      5  equilibria

 Phase region boundary   3 at:   5.361E-01  2.533E-02
     LIQUID
   ** ALCU_EPSILON
   ** BCC_B2

 Phase region boundary   4 at:   5.383E-01  3.569E-02
     LIQUID
   ** BCC_B2
 Calculated.                     12  equilibria

 Phase region boundary   5 at:   5.962E-01  1.431E-01
     LIQUID
  ** BCC_B2
   ** DIAMOND_A4

 Phase region boundary   6 at:   2.789E-01  5.911E-01
     LIQUID
   ** DIAMOND_A4
 Calculated                     41  equilibria

 Phase region boundary   7 at:   5.361E-01  2.533E-02
     LIQUID
   ** ALCU_EPSILON
 Calculated                     16  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      1  seconds

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   7.337E-01  2.597E-01
     LIQUID
  ** CU19SI6_ETA
 Calculated.                      4  equilibria

 Phase region boundary   2 at:   7.478E-01  2.387E-01
     LIQUID
   ** BCC_B2
   ** CU19SI6_ETA

 Phase region boundary   3 at:   7.525E-01  2.105E-01
     LIQUID
   ** BCC_B2
 Calculated.                      8  equilibria

 Phase region boundary   4 at:   6.917E-01  2.112E-01
     LIQUID
   ** BCC_B2
   ** DIAMOND_A4

 Phase region boundary   5 at:   3.329E-01  6.250E-01
     LIQUID
   ** DIAMOND_A4
 Calculated.                     14  equilibria

 Phase region boundary   6 at:   3.469E-01  6.529E-01
     LIQUID
   ** CU19SI6_ETA
   ** DIAMOND_A4

 Phase region boundary   7 at:   7.269E-01  2.729E-01
     LIQUID
   ** CU19SI6_ETA
 Calculated.                      6  equilibria
 Terminating at known equilibrium

 Phase region boundary   8 at:   7.337E-01  2.597E-01
     LIQUID
   ** CU19SI6_ETA
 Calculated.                      3  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      0  seconds
 T =  973.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.736E-01  5.113E-03
     LIQUID
  ** ALCU_EPSILON
```

```
 Calculated                      12  equilibria

 Phase region boundary   2 at:   4.736E-01  5.113E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated.                      11  equilibria

 Phase region boundary   3 at:   5.106E-01  6.209E-02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4

 Phase region boundary   4 at:   2.273E-01  5.621E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      36  equilibria

 Phase region boundary   5 at:   5.106E-01  6.209E-02
     LIQUID
  ** ALCU_EPSILON
 Calculated                      24  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      0  seconds
 T =  873.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   3.646E-02  1.803E-02
     LIQUID
  ** FCC_A1
 Calculated                      15  equilibria

 Phase region boundary   2 at:   3.646E-02  1.803E-02
     LIQUID
  ** FCC_A1
 Calculated                      33  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      0  seconds

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.151E-01  5.493E-03
     LIQUID
  ** ALCU_ETA
 Calculated                       8  equilibria

 Phase region boundary   2 at:   4.151E-01  5.493E-03
     LIQUID
  ** ALCU_ETA
 Calculated.                       6  equilibria

 Phase region boundary   3 at:   4.241E-01  3.756E-02
     LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA

 Phase region boundary   4 at:   4.398E-01  3.756E-02
     LIQUID
  ** ALCU_EPSILON
 Calculated.                       2  equilibria

 Phase region boundary   5 at:   4.420E-01  4.464E-02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4

 Phase region boundary   6 at:   1.706E-01  5.446E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      27  equilibria

 Phase region boundary   7 at:   4.241E-01  3.756E-02
     LIQUID
  ** ALCU_ETA
 Calculated                      17  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                      0  seconds
 T =  773.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 T = 1773.15 K
 Version R mapping is selected

 Organizing start points
```

```
Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   3.379E-01  7.512E-02  8.731E+02
     LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA
 CALCULATED     4 EQUILIBRIA

 Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA
     DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4
 CALCULATED    25 EQUILIBRIA

 Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
  ** ALCU_EPSILON
     BCC_B2
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
  ** ALCU_EPSILON
  ** BCC_B2
 Terminating at diagram limit
 CALCULATED    34 EQUILIBRIA

 Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
  ** BCC_B2
  ** DIAMOND_A4
 CALCULATED    43 EQUILIBRIA

 Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
  ** BCC_B2
     CU19SI6_ETA
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
  ** BCC_B2
  ** CU19SI6_ETA
 Terminating at known equilibrium
 CALCULATED    37 EQUILIBRIA

 Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
  ** CU19SI6_ETA
  ** DIAMOND_A4
 *** SORRY CANNOT CONTINUE ***    4

 CALCULATED    16 EQUILIBRIA

 Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_ETA
  ** DIAMOND_A4
 CALCULATED     9 EQUILIBRIA

 Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
  ** ALCU_ETA
     ALCU_THETA
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
  ** ALCU_ETA
  ** ALCU_THETA
 Terminating at diagram limit
 CALCULATED    14 EQUILIBRIA

 Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
  ** ALCU_THETA
  ** DIAMOND_A4
 CALCULATED    17 EQUILIBRIA

 Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
     LIQUID
  ** ALCU_THETA
  ** DIAMOND_A4
     FCC_A1
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
     LIQUID
  ** ALCU_THETA
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED    12 EQUILIBRIA

 Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
     LIQUID
  ** DIAMOND_A4
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED    21 EQUILIBRIA

 Phase region boundary   2 at:   3.379E-01  7.512E-02  8.731E+02
     LIQUID
  ** ALCU_EPSILON
```

```
  ** ALCU_ETA
 Terminating at diagram limit
 CALCULATED    12 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\LIQ
 UIDUS.POLY3
 CPU time for mapping                      0  seconds

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   8.482E-01  6.736E-02  1.273E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 *** SORRY CANNOT CONTINUE ***    9

 CALCULATED    46 EQUILIBRIA

 Phase region boundary   2 at:   8.482E-01  6.736E-02  1.273E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED    13 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\LIQ
 UIDUS.POLY3
 CPU time for mapping                      0  seconds

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   6.503E-01  8.154E-03  1.273E+03
     LIQUID
  ** BCC_B2
  ** GAMMA_H
 Terminating at diagram limit
 CALCULATED    13 EQUILIBRIA

 Phase region boundary   2 at:   6.503E-01  8.154E-03  1.273E+03
     LIQUID
  ** BCC_B2
  ** GAMMA_H
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\LIQ
 UIDUS.POLY3
 CPU time for mapping                      0  seconds
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
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 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4

 Phase region boundary   1 at:   8.482E-01  6.736E-02  1.273E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
```
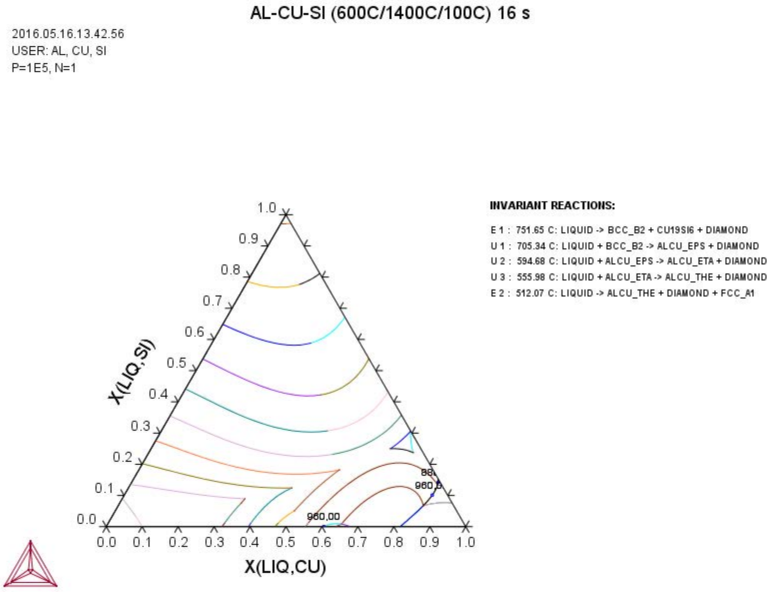

```
 *** SORRY CANNOT CONTINUE ***    9

 CALCULATED    46 EQUILIBRIA

 Phase region boundary   2 at:   8.482E-01  6.736E-02  1.273E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED    13 EQUILIBRIA

 Phase region boundary   2 at:   6.503E-01  8.154E-03  1.273E+03
     LIQUID
  ** BCC_B2
  ** GAMMA_H
 Terminating at diagram limit
 CALCULATED    13 EQUILIBRIA

 Phase region boundary   2 at:   6.503E-01  8.154E-03  1.273E+03
     LIQUID
  ** BCC_B2
  ** GAMMA_H
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
 OVAR.POLY3
 CPU time for mapping                     0  seconds
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Generating start point  31
 Generating start point  32

 Phase region boundary   1 at:   8.419E-01  6.666E-02
     LIQUID
  ** BCC_B2
 Calculated.                      28  equilibria

 Phase region boundary   2 at:   6.645E-01  6.795E-03
     LIQUID
  ** BCC_B2
  ** GAMMA_H

 Phase region boundary   3 at:   6.653E-01  4.077E-03
     LIQUID
  ** GAMMA_H
 Calculated                      12  equilibria

 Phase region boundary   4 at:   6.645E-01  6.795E-03
     LIQUID
  ** BCC_B2
 Calculated.                      26  equilibria

 Phase region boundary   5 at:   8.419E-01  6.666E-02
```

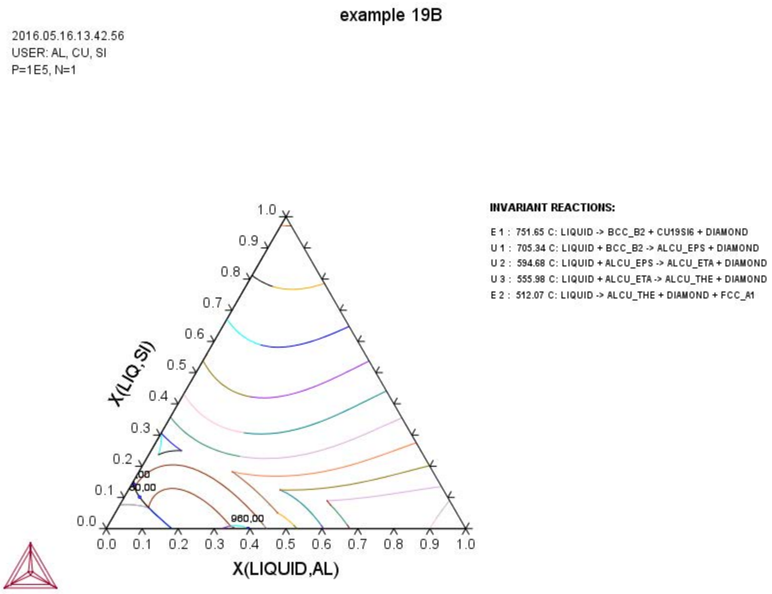
```
    LIQUID
 ** BCC_B2
 ** FCC_A1

Phase region boundary   6 at:   8.633E-01  4.917E-02
    LIQUID
 ** FCC_A1
Calculated                      25  equilibria

Phase region boundary   7 at:   8.633E-01  4.917E-02
    LIQUID
 ** FCC_A1
Calculated                      25  equilibria

Phase region boundary   8 at:   6.645E-01  6.795E-03
    LIQUID
 ** BCC_B2
Calculated.                      26  equilibria
Terminating at known equilibrium

Phase region boundary   9 at:   6.653E-01  4.077E-03
    LIQUID
 ** GAMMA_H
Calculated                      12  equilibria

Phase region boundary  10 at:   7.327E-03  9.853E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      15  equilibria

Phase region boundary  11 at:   7.327E-03  9.853E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      15  equilibria

Phase region boundary  12 at:   7.453E-02  8.883E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      23  equilibria

Phase region boundary  13 at:   7.453E-02  8.883E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      25  equilibria

Phase region boundary  14 at:   1.372E-01  7.942E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      30  equilibria

Phase region boundary  15 at:   1.372E-01  7.942E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      22  equilibria

Phase region boundary  16 at:   1.926E-01  7.111E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      28  equilibria

Phase region boundary  17 at:   1.926E-01  7.111E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      32  equilibria

Phase region boundary  18 at:   6.652E-01  9.329E-03
    LIQUID
 ** BCC_B2
Calculated.                       2  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   6.652E-01  9.329E-03
    LIQUID
 ** BCC_B2
Calculated.                      30  equilibria
Terminating at known equilibrium

Phase region boundary  20 at:   2.311E-01  6.535E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      34  equilibria

Phase region boundary  21 at:   2.311E-01  6.535E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      40  equilibria

Phase region boundary  22 at:   5.840E-01  7.591E-03
    LIQUID
 ** BCC_B2
Calculated                       9  equilibria

Phase region boundary  23 at:   5.840E-01  7.591E-03
    LIQUID
 ** BCC_B2
Calculated.                      39  equilibria

Phase region boundary  24 at:   8.543E-01  1.296E-01
    LIQUID
 ** BCC_B2
 ** FCC_A1

Phase region boundary  25 at:   8.749E-01  1.099E-01
    LIQUID
 ** FCC_A1
Calculated                      24  equilibria

Phase region boundary  26 at:   8.543E-01  1.296E-01
    LIQUID
 ** BCC_B2
Calculated                      54  equilibria

Phase region boundary  27 at:   2.562E-01  6.158E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      39  equilibria
```

```
Phase region boundary  28 at:   2.562E-01  6.158E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     37  equilibria

Phase region boundary  29 at:   5.198E-01  5.412E-03
    LIQUID
 ** ALCU_EPSILON
Calculated                     11  equilibria

Phase region boundary  30 at:   5.198E-01  5.412E-03
    LIQUID
 ** ALCU_EPSILON
Calculated.                      5  equilibria

Phase region boundary  31 at:   5.361E-01  2.533E-02
    LIQUID
 ** ALCU_EPSILON
 ** BCC_B2

Phase region boundary  32 at:   5.383E-01  3.569E-02
    LIQUID
 ** BCC_B2
Calculated.                     12  equilibria

Phase region boundary  33 at:   5.962E-01  1.431E-01
    LIQUID
 ** BCC_B2
 ** DIAMOND_A4

Phase region boundary  34 at:   2.789E-01  5.911E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     41  equilibria

Phase region boundary  35 at:   5.361E-01  2.533E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                     16  equilibria

Phase region boundary  36 at:   7.337E-01  2.597E-01
    LIQUID
 ** CU19SI6_ETA
Calculated.                      4  equilibria

Phase region boundary  37 at:   7.478E-01  2.387E-01
    LIQUID
 ** BCC_B2
 ** CU19SI6_ETA

Phase region boundary  38 at:   7.525E-01  2.105E-01
    LIQUID
 ** BCC_B2
Calculated.                      8  equilibria

Phase region boundary  39 at:   6.917E-01  2.112E-01
    LIQUID
 ** BCC_B2
 ** DIAMOND_A4

Phase region boundary  40 at:   3.329E-01  6.250E-01
    LIQUID
 ** DIAMOND_A4
Calculated.                     14  equilibria

Phase region boundary  41 at:   3.469E-01  6.529E-01
    LIQUID
 ** CU19SI6_ETA
 ** DIAMOND_A4

Phase region boundary  42 at:   7.269E-01  2.729E-01
    LIQUID
 ** CU19SI6_ETA
Calculated.                      6  equilibria
Terminating at known equilibrium

Phase region boundary  43 at:   7.337E-01  2.597E-01
    LIQUID
 ** CU19SI6_ETA
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  44 at:   4.736E-01  5.113E-03
    LIQUID
 ** ALCU_EPSILON
Calculated                     12  equilibria

Phase region boundary  45 at:   4.736E-01  5.113E-03
    LIQUID
 ** ALCU_EPSILON
Calculated.                     11  equilibria

Phase region boundary  46 at:   5.106E-01  6.209E-02
    LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4

Phase region boundary  47 at:   2.273E-01  5.621E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     36  equilibria

Phase region boundary  48 at:   5.106E-01  6.209E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                     24  equilibria

Phase region boundary  49 at:   3.646E-02  1.803E-02
    LIQUID
 ** FCC_A1
Calculated                     15  equilibria

Phase region boundary  50 at:   3.646E-02  1.803E-02
    LIQUID
 ** FCC_A1
```

```
Calculated                      33  equilibria

Phase region boundary  51 at:   4.151E-01  5.493E-03
    LIQUID
 ** ALCU_ETA
Calculated                       8  equilibria

Phase region boundary  52 at:   4.151E-01  5.493E-03
    LIQUID
 ** ALCU_ETA
Calculated.                       6  equilibria

Phase region boundary  53 at:   4.241E-01  3.756E-02
    LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA

Phase region boundary  54 at:   4.398E-01  3.756E-02
    LIQUID
 ** ALCU_EPSILON
Calculated.                       2  equilibria

Phase region boundary  55 at:   4.420E-01  4.464E-02
    LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4

Phase region boundary  56 at:   1.706E-01  5.446E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      27  equilibria

Phase region boundary  57 at:   4.241E-01  3.756E-02
    LIQUID
 ** ALCU_ETA
Calculated                      17  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping                      6  seconds

 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes


 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes


INVARIANT REACTIONS:

E 1:  751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1:  705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2:  594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3:  555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2:  512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1
```



```
POST: s-d-a x x(liquid,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 19B
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
INVARIANT REACTIONS:

E 1 :  751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1 :  705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2 :  594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3 :  555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2 :  512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1
```

```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex20

About

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex20\tcex20.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example showing how to calculate an adiabatic decompression
SYS: @@ using the geochemical database
SYS: @@
SYS: set-log ex20,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw user PGEO.TDB
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database

 O                       VA  DEFINED
 STEAM                   OXYGEN                  HYDROGEN
   REJECTED
 CARBON_MONOXIDE         CARBON_DIOXIDE          METHANE
   REJECTED
TDB_USER: d-sys mg si
   ... the command in full is DEFINE_SYSTEM
 MG                      SI  DEFINED
TDB_USER: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 GAS:G       :O2:
  > Gaseous Mixture with C-H-O species, using ideal gas model
 A_QUARTZ    :SI1O2:
 B_QUARTZ    :SI1O2:
 CRISTOBALITE :SI1O2:
 TRIDYMITE   :SI1O2:
 COESITE     :SI1O2:
 STISHOVITE  :SI1O2:
 PERICLASE   :MG1O1:
 FORSTERITE  :SI1MG2O4:
 BETA_FORSTERITE :SI1MG2O4:
 GAMMA_FORSTERITE :SI1MG2O4:
 ILMENITE_MG :SI1MG1O3:
 MG_PEROVSKITE :SI1MG1O3:
 CLINOENSTATITE :SI1MG1O3:
 ORTHOENSTATITE :SI1MG1O3:
 PROTOENSTATITE :SI1MG1O3:
 CLINOENSTHP :SI1MG1O3:
 GARNET_MG   :SI1MG1O3:
TDB_USER: rej ph gas proto
   ... the command in full is REJECT
 GAS:G                   PROTOENSTATITE  REJECTED
TDB_USER: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ We define more convenient components
POLY_3: def-com mgo o sio2
   ... the command in full is DEFINE_COMPONENTS
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 MGO                     ENTERED   SER
 O                       ENTERED   SER
 SIO2                    ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 TRIDYMITE               ENTERED      0.000000E+00    0.000000E+00
 STISHOVITE              ENTERED      0.000000E+00    0.000000E+00
 PERICLASE               ENTERED      0.000000E+00    0.000000E+00
 ORTHOENSTATITE          ENTERED      0.000000E+00    0.000000E+00
 MG_PEROVSKITE           ENTERED      0.000000E+00    0.000000E+00
 ILMENITE_MG             ENTERED      0.000000E+00    0.000000E+00
 GARNET_MG               ENTERED      0.000000E+00    0.000000E+00
 GAMMA_FORSTERITE        ENTERED      0.000000E+00    0.000000E+00
 FORSTERITE              ENTERED      0.000000E+00    0.000000E+00
 CRISTOBALITE            ENTERED      0.000000E+00    0.000000E+00
 COESITE                 ENTERED      0.000000E+00    0.000000E+00
 CLINOENSTHP             ENTERED      0.000000E+00    0.000000E+00
 CLINOENSTATITE          ENTERED      0.000000E+00    0.000000E+00
 B_QUARTZ                ENTERED      0.000000E+00    0.000000E+00
 BETA_FORSTERITE         ENTERED      0.000000E+00    0.000000E+00
 A_QUARTZ                ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 MG       ENTERED    O        ENTERED    SI1MG1O3 ENTERED    SIO2     ENTERED
 MG1O1    ENTERED    O2       ENTERED    SI1MG2O4 ENTERED    VA       ENTERED
 MGO      ENTERED    SI       ENTERED    SI1O2    ENTERED
POLY_3:Hit RETURN to continue
POLY_3: @@ and specify a composition assumed to be
POLY_3: @@ present in the earth mantle
POLY_3: s-i-a n(mgo)=80
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-i-a n(si1mg1o3)=100
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(MGO)=180, N(SIO2)=100
 DEGREES OF FREEDOM 3
```

```
POLY_3:Hit RETURN to continue
POLY_3: @@ There is an error if mgsio3 is used instead of the defined si1mg1o3,
POLY_3: @@ since mgsio3 is not defined as a species.
POLY_3: s-c t=2200,p=2e10
   ... the command in full is SET_CONDITION
POLY_3: save tcex20 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ We have no degree of freedom with respect
POLY_3: @@ to oxygen so set its activity to unity (or
POLY_3: @@ any positive number)
POLY_3: s-c ac(o)=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated            16 grid points in              0 s
    31 ITS,  CPU TIME USED   0 SECONDS
POLY_3: save tcex20 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 GARNET_MG              ENTERED      0.000000E+00    4.000000E+01
 BETA_FORSTERITE        ENTERED      0.000000E+00    2.400000E+02
 GAMMA_FORSTERITE       ENTERED     -5.946730E-03    0.000000E+00
 MG_PEROVSKITE          ENTERED     -2.558352E-02    0.000000E+00
 ILMENITE_MG            ENTERED     -4.828445E-02    0.000000E+00
 PERICLASE              ENTERED     -9.575143E-02    0.000000E+00
 CLINOENSTHP            ENTERED     -1.541632E-01    0.000000E+00
 ORTHOENSTATITE         ENTERED     -2.197450E-01    0.000000E+00
 CLINOENSTATITE         ENTERED     -2.394369E-01    0.000000E+00
 FORSTERITE             ENTERED     -2.417190E-01    0.000000E+00
 STISHOVITE             ENTERED     -3.053984E-01    0.000000E+00
 COESITE                ENTERED     -3.775316E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -7.835592E+00
 A_QUARTZ B_QUARTZ TRIDYMITE CRISTOBALITE
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: X
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 N(MGO)=180, N(SIO2)=100, T=2200, P=2E10, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature   2200.00 K (  1926.85 C),  Pressure  2.000000E+10
 Number of moles of components  2.80000E+02,  Mass in grams  1.32632E+04
 Total Gibbs energy -1.80863E+08,  Enthalpy -9.91578E+07,  Volume  3.55512E-03

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 MGO                     1.8000E+02  6.4286E-01 7.6674E-14 -5.5240E+05 SER
 O                       0.0000E+00  0.0000E+00 1.0000E+00  0.0000E+00 SER
 SIO2                    1.0000E+02  3.5714E-01 4.6393E-20 -8.1430E+05 SER

 BETA_FORSTERITE             Status ENTERED     Driving force  0.0000E+00
 Moles 2.4000E+02, Mass 1.1255E+04, Volume fraction 8.5320E-01  Mole fractions:
 MGO   6.66667E-01  SIO2  3.33333E-01  O     0.00000E+00

 GARNET_MG                   Status ENTERED     Driving force  0.0000E+00
 Moles 4.0000E+01, Mass 2.0078E+03, Volume fraction 1.4680E-01  Mole fractions:
 MGO   5.00000E-01  SIO2  5.00000E-01  O     0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: ent fun dens=1e-3*bm/vm;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh dens
   ... the command in full is SHOW_VALUE
 DENS=3730.7358
POLY_3: @@ We have now found the equilibrium at this
POLY_3: @@ pressure. Now assume this system is decompressed
POLY_3: @@ adiabatically. What will the new temperature become?
POLY_3: s-c h
   ... the command in full is SET_CONDITION
Value /-99157833.21/:
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /2200/: none
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(MGO)=180, N(SIO2)=100, P=2E10, AC(O)=1, H=-9.91578E7
 DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: @@ Now t is independent, calculate the equilibrium and get t
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=2200.
POLY_3:Hit RETURN to continue
POLY_3: @@ No big surprise! the same temperature. Now change pressure
POLY_3: s-c p
   ... the command in full is SET_CONDITION
Value /2E+10/: 150e8
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated            16 grid points in              0 s
    18 ITS,  CPU TIME USED   0 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=2977.6276
POLY_3:Hit RETURN to continue
POLY_3: @@ We will also have a new density and another set of
POLY_3: @@ stable phases.
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
```

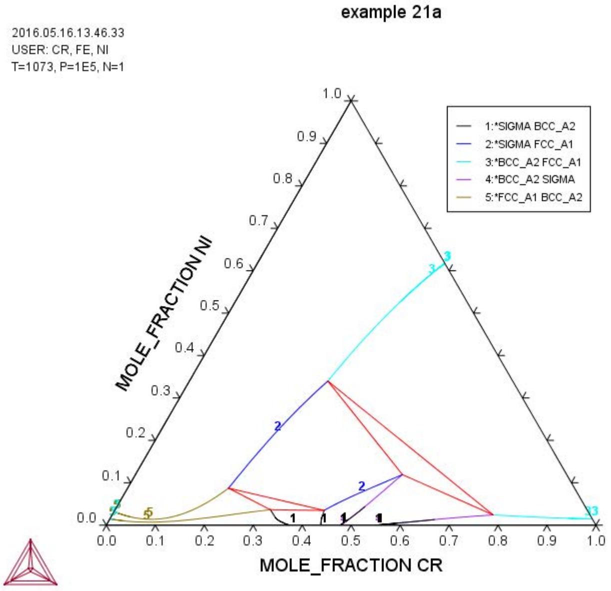
```
Options /VXCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 N(MGO)=180, N(SIO2)=100, P=1.5E10, AC(O)=1, H=-9.91578E7
 DEGREES OF FREEDOM 0

 Temperature   2977.63 K (  2704.48 C),  Pressure  1.500000E+10
 Number of moles of components  2.80000E+02,  Mass in grams  1.32632E+04
 Total Gibbs energy -2.30661E+08,  Enthalpy -9.91578E+07,  Volume  3.59115E-03

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 MGO                     1.8000E+02  6.4286E-01 4.6875E-13 -7.0283E+05 SER
 O                       0.0000E+00  0.0000E+00 1.0000E+00  0.0000E+00 SER
 SIO2                    1.0000E+02  3.5714E-01 5.3688E-19 -1.0415E+06 SER

 GARNET_MG                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.0000E+02, Mass 1.0039E+04, Volume fraction 7.4847E-01  Mole fractions:
 MGO   5.00000E-01  SIO2  5.00000E-01  O     0.00000E+00

 PERICLASE                   Status ENTERED     Driving force  0.0000E+00
 Moles 8.0000E+01, Mass 3.2244E+03, Volume fraction 2.5153E-01  Mole fractions:
 MGO   1.00000E+00  SIO2  0.00000E+00  O     0.00000E+00
POLY_3: sh dens
   ... the command in full is SHOW_VALUE
 DENS=3693.3029
POLY_3: sh v
   ... the command in full is SHOW_VALUE
 V=3.5911547E-3
POLY_3: sh vm
   ... the command in full is SHOW_VALUE
 VM=1.2825553E-5
POLY_3:
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3:
```

tcex21

```
About License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex21\tcex21.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Demonstrates the use of a user-defined database, calculate a ternary isotherm in Fe-Cr-Ni.
SYS: @@
SYS: @@
SYS: set-log ex21,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw user tcex21
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
TDB_USER: def-sys *
   ... the command in full is DEFINE_SYSTEM
 /-                      VA                      CR
 FE                      NI  DEFINED
TDB_USER: li-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 LIQUID:L    :CR FE NI:
 BCC_A2      :CR FE NI:VA:
 FCC_A1      :CR FE NI:VA:
 HCP_A3      :CR FE NI:VA:
 SIGMA       :FE NI:CR:CR FE NI:
TDB_USER:Hit RETURN to continue
TDB_USER: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A.T. Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4, p 317-425; '
  'J.O. Andersson, B. Sundman, Calphad 11(1987)1 p 83-92 TRITA-MAC 270
      (1986); Cr-Fe'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'Byeong-Joo Lee, Calphad 16(1992)2, p 121-149; carbides'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Fe-Ni'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Cr-Ni'
  'A.F. Guillermet, Z. Metallkde. 79(1988)8 p 524-536, TRITA-MAC 362 (1988);
      C-Co-Ni, C-Co-Fe-Ni'
  'K. Frisk, Metall. Trans. 21A (1990)9 p 2477-2488, Cr-Fe-N'
  'Unassessed parameter, linear combination of unary data.'
  'P. Gustafson, Calphad 12(1987)3 p 277-292, Cr-Ni-W '
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ With 3 components we must set 5 conditions
POLY_3: s-c t=1073 p=1e5 n=1 x(cr)=.2 x(ni)=.2
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1073, P=1E5, N=1, X(CR)=0.2, X(NI)=0.2
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          9315 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1073, P=1E5, N=1, X(CR)=0.2, X(NI)=0.2
 DEGREES OF FREEDOM 0

 Temperature   1073.00 K (   799.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.56454E+01
 Total Gibbs energy -5.39559E+04,  Enthalpy  3.01555E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      2.0000E-01  1.8688E-01 5.8626E-03 -4.5849E+04 SER
 FE                      6.0000E-01  6.0217E-01 3.1002E-03 -5.1533E+04 SER
 NI                      2.0000E-01  2.1094E-01 4.2164E-04 -6.9332E+04 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.5645E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  6.02174E-01  NI  2.10943E-01  CR  1.86883E-01
POLY_3:Hit RETURN to continue
POLY_3: @@ Define axis
POLY_3: s-a-v 1 x(cr) 0 1,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(ni) 0 1,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex21 y
   ... the command in full is SAVE_WORKSPACES
```

```
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 ERROR                   1611  when calculating equilibrium
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18

 Phase region boundary   1 at:   3.521E-02  1.510E-02
     BCC_A2
  ** FCC_A1
 Calculated.                      20  equilibria

 Phase region boundary   2 at:   2.615E-01  6.190E-02
     BCC_A2
  ** FCC_A1
  ** SIGMA

 Phase region boundary   3 at:   3.723E-01  3.566E-02
     BCC_A2
  ** SIGMA
 Calculated                      21  equilibria

 Phase region boundary   4 at:   3.168E-01  6.107E-02
     FCC_A1
  ** SIGMA
 Calculated.                      20  equilibria

 Phase region boundary   5 at:   4.140E-01  2.295E-01
  ** BCC_A2
     FCC_A1
  ** SIGMA

 Phase region boundary   6 at:   5.304E-01  1.820E-01
  ** BCC_A2
     FCC_A1
 Calculated                      43  equilibria

 Phase region boundary   7 at:   6.616E-01  7.178E-02
  ** BCC_A2
     SIGMA
 Calculated                      31  equilibria

 Phase region boundary   8 at:   2.615E-01  6.190E-02
     BCC_A2
  ** FCC_A1
 Calculated                      33  equilibria

 Phase region boundary   9 at:   3.521E-02  1.510E-02
     BCC_A2
  ** FCC_A1
 Calculated                      15  equilibria

 Phase region boundary  10 at:   1.095E-02  2.044E-02
     BCC_A2
  ** FCC_A1
 Calculated                      18  equilibria

 Phase region boundary  11 at:   1.095E-02  2.044E-02
     BCC_A2
  ** FCC_A1
 Calculated.                      22  equilibria
 Terminating at known equilibrium

 Phase region boundary  12 at:   3.838E-01  1.780E-02
     BCC_A2
  ** SIGMA
 Calculated.                       2  equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   3.838E-01  1.780E-02
     BCC_A2
  ** SIGMA
 Calculated                      21  equilibria

 Phase region boundary  14 at:   5.848E-01  2.838E-02
     BCC_A2
  ** SIGMA
 Calculated                      32  equilibria

 Phase region boundary  15 at:   5.848E-01  2.838E-02
     BCC_A2
  ** SIGMA
 Calculated.                       8  equilibria
 Terminating at known equilibrium

 Phase region boundary  16 at:   5.404E-01  9.033E-03
```

```
     BCC_A2
  ** SIGMA
 Calculated                     12  equilibria

 Phase region boundary  17 at:   5.404E-01  9.033E-03
     BCC_A2
  ** SIGMA
 Calculated.                     13  equilibria
 Terminating at known equilibrium

 Phase region boundary  18 at:   4.123E-01  2.273E-01
     FCC_A1
  ** SIGMA
 Calculated.                     19  equilibria
 Terminating at known equilibrium

 Phase region boundary  19 at:   4.123E-01  2.273E-01
     FCC_A1
  ** SIGMA
 Calculated.                      2  equilibria
 Terminating at known equilibrium

 Phase region boundary  20 at:   9.183E-03  2.090E-02
  ** BCC_A2
     FCC_A1
 Calculated                     13  equilibria

 Phase region boundary  21 at:   9.183E-03  2.090E-02
  ** BCC_A2
     FCC_A1
 Calculated.                     22  equilibria
 Terminating at known equilibrium

 Phase region boundary  22 at:   6.363E-01  2.710E-01
  ** BCC_A2
     FCC_A1
 Calculated.                     16  equilibria
 Terminating at known equilibrium

 Phase region boundary  23 at:   6.363E-01  2.710E-01
  ** BCC_A2
     FCC_A1
 Calculated                     26  equilibria

 Phase region boundary  24 at:   6.789E-01  3.114E-01
  ** BCC_A2
     FCC_A1
 Calculated.                     22  equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   6.789E-01  3.114E-01
  ** BCC_A2
     FCC_A1
 Calculated                     16  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex21\tcex
 21.POLY3
 CPU time for mapping                       1  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST: set-title example 21a
POST: se-d-ty y,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-l b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex22

About

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex22\tcex22.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of a heat balance. In this case C3H8 is burned in
SYS: @@ oxygen and the adiabatic flame temperature is calculated.
SYS: @@
SYS: set-log ex22,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw ssub5
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v5.1

 VA  DEFINED
TDB_SSUB5: def-sys c o h
   ... the command in full is DEFINE_SYSTEM
 C                       O                       H
   DEFINED
TDB_SSUB5: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
      C1<G> C<G>
   C1H1<G> T.C.R.A.S. Class: 2
      C1H1<G> CH<G>
   C1H1O1<G> T.C.R.A.S. Class: 4
      C1H1O1<G> HCO<G>
      FORMYL <GAS>
   C1H1O2<G> T.C.R.A.S. Class: 6
      C1H1O2<G>
   C1H2<G> T.C.R.A.S. Class: 5
      C1H2<G> CH2<G> METHYLENE
      METHYLENE <GAS>
   C1H2O1<G> T.C.R.A.S. Class: 5
      C1H2O1<G> CH2O<G>
      FORMALDEHYDE <GAS>
   C1H2O2_CIS<G> T.C.R.A.S. Class: 5
      C1H2O2_CIS<G>
   C1H2O2_DIOXIRANE<G> T.C.R.A.S. Class: 6
      C1H2O2_DIOXIRANE<G>
      S298 corrected and cp refitted
      due to corrected data in IVTAN2000 7/2002
   C1H2O2_TRANS<G> T.C.R.A.S. Class: 5
      C1H2O2_TRANS<G>
   C1H3<G> T.C.R.A.S. Class: 5
      C1H3<G> CH3<G>
      METHYL, Gaseous Standard State.
   C1H3O1_CH2OH<G> T.C.R.A.S. Class: 6
      C1H3O1_CH2OH<G>
   C1H3O1_CH3O<G> T.C.R.A.S. Class: 5
      C1H3O1_CH3O<G>
   C1H4<G> T.C.R.A.S. Class: 5
      C1H4<G> CH4<G> METHANE
      METHANE, Gaseous Standard State.
   C1H4O1<G> T.C.R.A.S. Class: 5
      C1H4O1<G> CH3OH<G>
      METHANOL <GAS>
   C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      C1O1<G> CO<G>
      CARBON MONOXIDE <GAS>
      STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
   C1O2<G> T.C.R.A.S. Class: 2
      C1O2<G> CO2<G>
      CARBON DIOXIDE <GAS>
   C2<G> T.C.R.A.S. Class: 2
      C2<G>
      CARBON Diatomic Gas.
   C2H1<G> T.C.R.A.S. Class: 6
      C2H1<G> C2H<G>
      CCH RADICAL <GAS>
   C2H2<G> T.C.R.A.S. Class: 2
      C2H2<G>
      ACETYLENE (ETYNE). Gaseous Standard State.
   C2H2O1<G> T.C.R.A.S. Class: 6
      C2H2O1<G>
      OXIRENE
      S298 corrected and cp refitted
      due to corrected data in IVTAN2000 7/2002
   C2H3<G> T.C.R.A.S. Class: 6
      C2H3<G>
      DICARBON TRIHYDRIDE, Gaseous Standard State.
   C2H4<G> T.C.R.A.S. Class: 6
      C2H4<G>
      ETHYLENE. Gaseous Standard State.
   C2H4O1_ACETALDEHYDE<G> T.C.R.A.S. Class: 5
      C2H4O1_ACETALDEHYDE<G>
   C2H4O1_OXIRANE<G> T.C.R.A.S. Class: 6
      C2H4O1_OXIRANE<G>
      S298 corrected and cp refitted
      due to corrected data in IVTAN2000 7/2002
   C2H4O2_ACETICACID<G> T.C.R.A.S. Class: 5
      C2H4O2_ACETICACID<G>
   C2H4O2_DIOXETANE<G> T.C.R.A.S. Class: 6
      C2H4O2_DIOXETANE<G>
      S298 corrected and cp refitted
      due to corrected data in IVTAN2000 7/2002
```

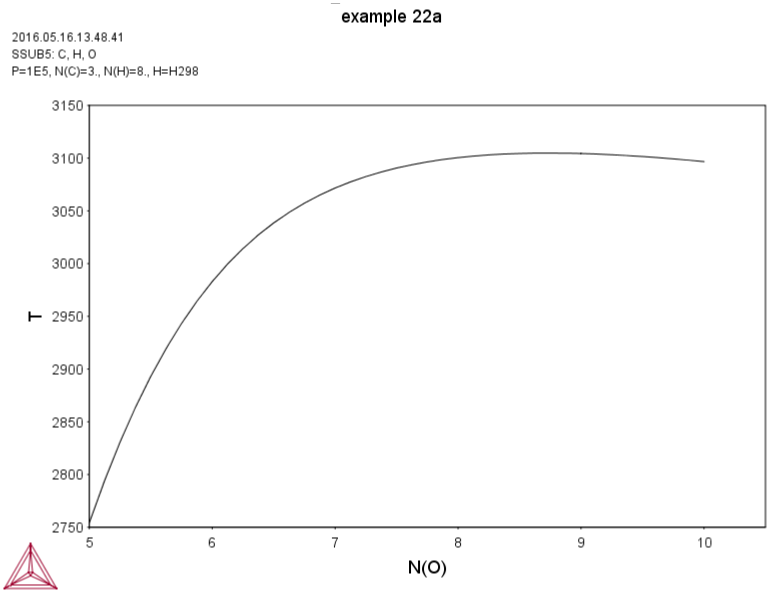
```
   typing error corrected 12/06
C2H4O3_123TRIOXOLANE<G> T.C.R.A.S. Class: 7
   C2H4O3_123TRIOXOLANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C2H4O3_124TRIOXOLANE<G> T.C.R.A.S. Class: 7
   C2H4O3_124TRIOXOLANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
   typing error corrected 12/06
C2H5<G> T.C.R.A.S. Class: 6
   C2H5<G>
   ETHYL radical. Gaseous Standard State.
C2H6<G> T.C.R.A.S. Class: 6
   C2H6<G>
   ETHANE. Gaseous Standard State.
C2H6O1<G> T.C.R.A.S. Class: 6
   C2H6O1<G> C2H6O<G>
   ETHANOL <GAS>
C2H6O2<G> THERMODATA
   C2H6O2<G>
   E-GLYCOL <GAS>.Data revised by THDA.
C2O1<G> T.C.R.A.S. Class: 5
   C2O1<G> C2O<G>
C3<G> T.C.R.A.S. Class: 6
   C3<G>
   CARBON <TRIATOMIC GAS>
C3H1<G> T.C.R.A.S. Class: 6
   C3H1<G> C3H<G>
   2-PROPYNYLIDYNE (gaseous state)
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C3H4_1<G> STULL WESTRUM SINKE 1969 SGTE
   C3H4_1<G>
   ALLENE = 1,2-PROPADIENE (gaseous state)
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H4_2<G> STULL WESTRUM SINKE 1969 SGTE
   C3H4_2<G>
   PROPYNE (METHYLACETYLENE) (gaseous state)
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H6O1<G> THERMODATA 01/93
   C3H6O1<G> ACETONE gas
   ACETONE (gaseous state)
   28/01/93
C3H6_1<G> T.C.R.A.S. Class: 6 4.09.85
   C3H6_1<G> Cyclopropane gas
C3H6_2<G> STULL WESTRUM SINKE 1969 SGTE
   C3H6_2<G> PROPENE gas
   PROPENE (gaseous state)
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H8<G> THERMODATA SGTE
   C3H8<G> PROPANE gas
   PROPANE <Gaseous Standard State>
C3O2<G> T.C.R.A.S. Class: 6
   C3O2<G>
C4<G> T.C.R.A.S. Class: 7
   C4<G>
C4H1<G> T.C.R.A.S Class: 6
   C4H1<G> C4H<G> 1,3-BUTADIYNYL gas
   1,3-BUTADIYNYL (Gaseous Standard State).
   Data provided by T.C.R.A.S. in 2000
C4H10_1<G> T.C.R.A.S Class: 4
   C4H10_1<G> BUTANE gas
   BUTANE (Gaseous Standard State).
   Data provided by T.C.R.A.S. in 2000
C4H10_2<G> T.C.R.A.S Class: 4
   C4H10_2<G> METHYLPROPANE N-BUTANE gas
   METHYLPROPANE N-BUTANE (Gaseous Standard State).
   Data provided by T.C.R.A.S. in 2000
C4H2_1<G> THERMODATA 1978 ST
   C4H2_1<G> 1,3-BUTADIYNE gas
C4H2_2<G> THERMODATA 06/93 ST
   C4H2_2<G> BUTADIYNE (BIACETYLENE) gas
C4H4_1<G> T.C.R.A.S Class: 6
   C4H4_1<G> 1,3-CYCLOBUTADIENE gas.
   1,3-CYCLOBUTADIENE. Gaseous Standard State.
   Data provided by T.C.R.A.S. in 2000
C4H4_2<G> STULL WESTRUM SINKE 1969 SGTE
   C4H4_2<G> 1-BUTEN-3-YNE VINYLACETYLENE gas
   1-BUTEN-3-YNE VINYLACETYLENE. Gaseous Standard State.
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_1<G> STULL WESTRUM SINKE 1969 SGTE
   C4H6_1<G>
   1,2-BUTADIENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_2<G> STULL WESTRUM SINKE 1969 SGTE
   C4H6_2<G>
   1,3-BUTADIENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_3<G> STULL WESTRUM SINKE 1969 SGTE
   C4H6_3<G>
   1-BUTYNE ETHYLACETYLENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_4<G> STULL WESTRUM SINKE 1969 SGTE
   C4H6_4<G>
   2-BUTYNE DIMETHYLACETYLENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_5<G> T.C.R.A.S Class: 6
   C4H6_5<G>
   CYCLOBUTENE. Data provided by T.C.R.A.S. in 2000
C4H8_1<G> THERMODATA 04/98 TC
   C4H8_1<G> 1-BUTENE gas
C4H8_2<G> THERMODATA 04/98 TC
   C4H8_2<G> (E)-2-BUTENE gas
C4H8_3<G> THERMODATA 04/98 TC
   C4H8_3<G> (Z)-2-BUTENE gas
C4H8_4<G> THERMODATA 04/98 TC
   C4H8_4<G> CYCLOBUTANE gas
C4H8_5<G> THERMODATA 04/98 TC
   C4H8_5<G> 2-METHYLPROPENE gas
C4H8_6<G> THERMODATA 04/98 TC
   C4H8_6<G> METHYLCYCLOPROPANE gas
C5<G> T.C.R.A.S. Class: 7
   C5<G>
C60<G> MHR-95
   C60<G>
```

```
      Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
      J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the rotational
      data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that
      a frequency with degeneracy 5 is missing from list in [94Kor/Sid];
      taken to be 419 cm-1, which gives very good, though not exact,
      agreement with values quoted in [94Kor/Sid]. Note discrepancy
      between calculated DrS(298) = -8943.5 J mol K-1 for the reaction
      60C<g>=C60<g>and that given by [94Kor/Sid] in their Table 5,
      -8950 J mol K-1. Enthalpy of formation: DfH = 2588 kJ/mol from
      DsubH(298.15K) = 166 +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure
      values reproduced very well.
      [91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).
   C6H6<G> T.C.R.A.S Class: 5
      C6H6<G> BENZENE gas
      BENZENE (Gaseous Standard State).
      Data provided by T.C.R.A.S. in 2000
   C6H6O1<G> THERMODATA 01/93
      C6H6O1<G>
      PHENOL gas
      28/01/93
   H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
      H1<G> H<G>
      HYDROGEN <MONATOMIC GAS>
   H1O1<G> T.C.R.A.S. Class: 1
      H1O1<G> OH<G>
   H1O2<G> T.C.R.A.S. Class: 4
      H1O2<G> HO2<G>
   H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      H2<G> H2<G>
      HYDROGEN<G>
      STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   H2O1<G> T.C.R.A.S. Class: 1
      H2O1<G> H2O<G>
      WATER <GAS>, STEAM
   H2O2<G> JANAF SECOND EDIT SGTE
      H2O2<G> H2O2<G>
      HYDROGEN PEROXIDE <GAS>
   O1<G> TCRAS 02/06/80
      O1<G> O<G>
   O2<G> TCRAS 21/06/90
      O2<G>
      OXYGEN Gaseous Standard State.
   O3<G> TCRAS 02/06/80
      O3<G>
      OZONE Gaseous Standard State.
   C1H2O2<L> THERMODATA 01/93
      C1H2O2_Liquid HCOOH_Liquid
      FORMIC ACID MONOMERIC
      28/01/93
   C1H4O1<L> I. BARIN 3rd. Edition
      C1H4O1_Liquid CH3OH_Liquid
      METHANOL (Liquid). H298 and S298 modified.
   C2H4O2<L> THERMODATA 01/93
      C2H4O2_Liquid
      ACETIC ACID (Liquid)
      28/01/93 Tb=389K.
   C2H6O1<L> THERMODATA 01/93
      C2H6O1_Liquid C2H6O_Liquid
      ETHANOL (Liquid)
      28/01/93
   C2H6O2<L> THERMODATA
      C2H6O2_Liquid
      E-GLYCOL (Liquid)
      Data revised by THDA.
   C60 MHR-95
      C60
      Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.
      The
      Fitted to the data in [94Kor/Sid], who took the phase transition at
      257K
      that [94Kor/Sid] do not give an explicit value for S(298.15K).
      S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =425.8 and Cp
      e
      calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]
      in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.
      Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
      the value preferred, if obliquely, by [94Kor/Sid].
      [92Ste/Chi]W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,
      P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).
   C6H6<L> THERMODATA 04/99 BC
      C6H6_Liquid BENZENE Liquid
   C1<DIAMOND> S.G.T.E. **
      C_DIAMOND
      <DIAMOND>
      Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
      from 1994 database (ex THERMODATA 01/93)
   C1<GRAPHITE> S.G.T.E. **
      C_GRAPHITE
      Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
   H2O1<L> T.C.R.A.S. Class: 4
      H2O1_Liquid H2O_Liquid Pure_Water
      WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002
   H2O2<L> THERMODATA 01/93
      H2O2_Liquid H2O2_Liquid
      HYDROGEN PEROXIDE
      28/01/93
 -OK-
TDB_SSUB5: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 C                        ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 H2O2_L                   ENTERED      0.000000E+00    0.000000E+00
 H2O1_L                   ENTERED      0.000000E+00    0.000000E+00
 GRAPHITE_L               ENTERED      0.000000E+00    0.000000E+00
```

```
 GRAPHITE                ENTERED      0.000000E+00    0.000000E+00
 DIAMOND                 ENTERED      0.000000E+00    0.000000E+00
 C6H6_L                  ENTERED      0.000000E+00    0.000000E+00
 C60_S                   ENTERED      0.000000E+00    0.000000E+00
 C2H6O2_L                ENTERED      0.000000E+00    0.000000E+00
 C2H6O1_L                ENTERED      0.000000E+00    0.000000E+00
 C2H4O2_L                ENTERED      0.000000E+00    0.000000E+00
 C1H4O1_L                ENTERED      0.000000E+00    0.000000E+00
 C1H2O2_L                ENTERED      0.000000E+00    0.000000E+00
 GAS                     ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 C                    ENTERED    C3H6O1               ENTERED
 C1H1                 ENTERED    C3H6_1               ENTERED
 C1H1O1               ENTERED    C3H6_2               ENTERED
 C1H1O2               ENTERED    C3H8                 ENTERED
 C1H2                 ENTERED    C3O2                 ENTERED
 C1H2O1               ENTERED    C4                   ENTERED
 C1H2O2               ENTERED    C4H1                 ENTERED
 C1H2O2_CIS           ENTERED    C4H10_1              ENTERED
 C1H2O2_DIOXIRANE     ENTERED    C4H10_2              ENTERED
 C1H2O2_TRANS         ENTERED    C4H2_1               ENTERED
 C1H3                 ENTERED    C4H2_2               ENTERED
 C1H3O1_CH2OH         ENTERED    C4H4_1               ENTERED
 C1H3O1_CH3O          ENTERED    C4H4_2               ENTERED
 C1H4                 ENTERED    C4H6_1               ENTERED
 C1H4O1               ENTERED    C4H6_2               ENTERED
 C1O1                 ENTERED    C4H6_3               ENTERED
 C1O2                 ENTERED    C4H6_4               ENTERED
 C2                   ENTERED    C4H6_5               ENTERED
 C2H1                 ENTERED    C4H8_1               ENTERED
 C2H2                 ENTERED    C4H8_2               ENTERED
 C2H2O1               ENTERED    C4H8_3               ENTERED
 C2H3                 ENTERED    C4H8_4               ENTERED
 C2H4                 ENTERED    C4H8_5               ENTERED
 C2H4O1_ACETALDEHYDE  ENTERED    C4H8_6               ENTERED
 C2H4O1_OXIRANE       ENTERED    C5                   ENTERED
 C2H4O2               ENTERED    C60                  ENTERED
 C2H4O2_ACETICACID    ENTERED    C6H6                 ENTERED
 C2H4O2_DIOXETANE     ENTERED    C6H6O1               ENTERED
 C2H4O3_123TRIOXOLANE ENTERED    H                    ENTERED
 C2H4O3_124TRIOXOLANE ENTERED    H1O1                 ENTERED
 C2H5                 ENTERED    H1O2                 ENTERED
 C2H6                 ENTERED    H2                   ENTERED
 C2H6O1               ENTERED    H2O1                 ENTERED
 C2H6O2               ENTERED    H2O2                 ENTERED
 C2O1                 ENTERED    O                    ENTERED
 C3                   ENTERED    O2                   ENTERED
 C3H1                 ENTERED    O3                   ENTERED
 C3H4_1               ENTERED    VA                   ENTERED
 C3H4_2               ENTERED
POLY_3: @@ We need to know the heat content of C3H8<G> at room temperature.
POLY_3: @@ This is a simple number to look up in a table but actually quite
POLY_3: @@ tricky to calculate as pure C3H8 at room temperature does not
POLY_3: @@ represent an equilibrium state. However, one can obtain it by
POLY_3: @@ the following procedure.
POLY_3: s-c t=298.15,p=1e5,n(o)=1e-10
   ... the command in full is SET_CONDITION
POLY_3: s-i-a n(c3h8)=1
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: c-s p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-s p gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated             74 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ The equilibrium state at room temperature is listed
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB5

 Conditions:
 T=298.15, P=1E5, N(O)=1E-10, N(C)=3, N(H)=8
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.10000E+01,  Mass in grams  4.40962E+01
 Total Gibbs energy -2.20108E+05,  Enthalpy -1.06064E+05,  Volume  4.99502E-02

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.0000E+00  8.1715E-01 1.1356E+07  4.0271E+04 SER
 H                       8.0000E+00  1.8285E-01 3.4211E-08 -4.2615E+04 SER
 O                       1.0000E-10  3.6282E-11 1.2651E-49 -2.7911E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.1000E+01, Mass 4.4096E+01, Volume fraction 1.0000E+00  Mass fractions:
 C  8.17145E-01  H  1.82855E-01  O  3.62820E-11
 Constitution:
 C1H4         9.90348E-01  C2H6O1       1.83029E-24  C4H6_3       1.00000E-30
 C60          8.16678E-03  C1H4O1       1.08754E-24  C2H4O1_OXIRA 1.00000E-30
 C6H6         1.38456E-03  C1H2O1       4.96084E-27  C4H6_5       1.00000E-30
 C2H6         1.00313E-04  C1H2O2_CIS   4.88436E-27  C5           1.00000E-30
 C3H8         5.44582E-07  C4H6_4       3.94602E-28  C2H3         1.00000E-30
 C4H10_2      3.84975E-08  C3H4_2       6.04110E-29  C2H2O1       1.00000E-30
 H2           7.83769E-09  C2H5         1.32230E-29  C2H2         1.00000E-30
 C4H10_1      6.16323E-09  C1H2O2_TRANS 6.61825E-30  C2H1         1.00000E-30
 C1O2         2.32090E-11  C3H4_1       2.45341E-30  C2           1.00000E-30
 H2O1         2.50979E-12  C4H6_1       2.07866E-30  H            1.00000E-30
 C1O1         7.01016E-13  C            1.00000E-30  H1O1         1.00000E-30
 C4H8_5       6.29486E-14  C3O2         1.00000E-30  H1O2         1.00000E-30
 C3H6_2       5.52670E-14  C4           1.00000E-30  H2O2         1.00000E-30
 C2H4         3.33175E-14  C4H1         1.00000E-30  C1H3O1_CH3O  1.00000E-30
 C4H8_2       7.83367E-15  C4H2_1       1.00000E-30  C1H3O1_CH2OH 1.00000E-30
 C4H8_3       3.33692E-15  C3H1         1.00000E-30  C1H3         1.00000E-30
 C4H8_1       4.53470E-16  C3           1.00000E-30  O            1.00000E-30
 C6H6O1       1.02341E-18  C2O1         1.00000E-30  C1H2O2_DIOXI 1.00000E-30
 C3H6O1       9.99430E-20  C2H6O2       1.00000E-30  O2           1.00000E-30
 C3H6_1       2.70389E-21  C4H2_2       1.00000E-30  O3           1.00000E-30
 C4H8_6       1.07592E-21  C4H4_1       1.00000E-30  C1H2         1.00000E-30
 C4H6_2       4.91032E-22  C4H4_2       1.00000E-30  C1H1O2       1.00000E-30
```

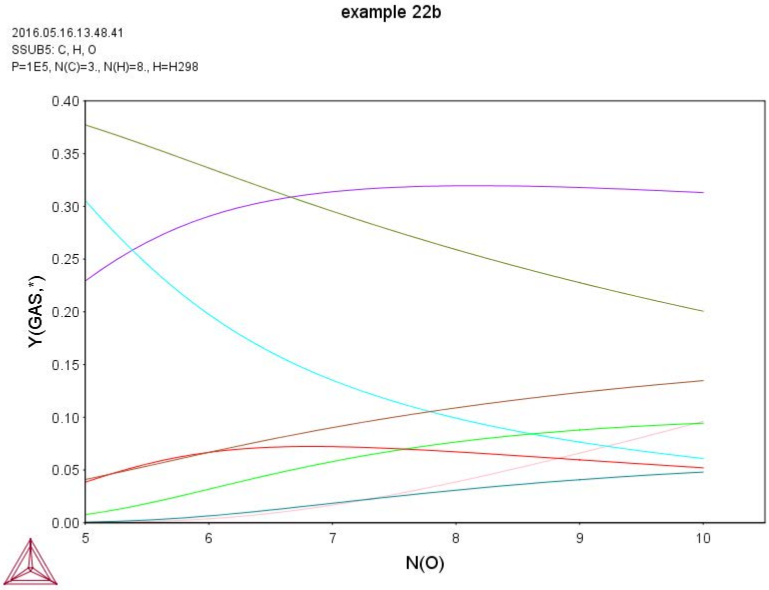
```
 C2H4O1_ACETA 1.25014E-22  C2H4O3_124TR 1.00000E-30  C1H1O1       1.00000E-30
 C4H8_4       2.10624E-23  C2H4O3_123TR 1.00000E-30  C1H1         1.00000E-30
 C2H4O2_ACETI 9.64309E-24  C2H4O2_DIOXE 1.00000E-30
POLY_3: @@ The enthalpy for the system is
POLY_3: sh h
   ... the command in full is SHOW_VALUE
 H=-106064.27
POLY_3:Hit RETURN to continue
POLY_3: @@ But we want a gas with just C3H8. Use the set-all-startvalues command.
POLY_3: s-a-s
   ... the command in full is SET_ALL_START_VALUES
Automatic start values for phase constituents? /N/: n

Should GAS be stable? /Y/: 1
Major constituent(s): C3H8
POLY_3: sh h
   ... the command in full is SHOW_VALUE
 H=-99369.211
POLY_3: @@ The difference in H for the two calculations is actually not very large.
POLY_3: @@ The value is approximate but rather good as the enthalpy is calculated
POLY_3: @@ for the following gas constitution
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB5

 Conditions:
 T=298.15, P=1E5, N(O)=1E-10, N(C)=3, N(H)=8
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.07452E+01,  Mass in grams  4.32989E+01
 Total Gibbs energy -1.78514E+05,  Enthalpy -9.93692E+04,  Volume  2.43004E-02

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.9419E+00  8.1606E-01 1.1356E+07  4.0271E+04 SER
 H                       7.7967E+00  1.8149E-01 3.4211E-08 -4.2615E+04 SER
 O                       6.6216E-03  2.4467E-03 1.2651E-49 -2.7911E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0745E+01, Mass 4.3299E+01, Volume fraction 1.0000E+00  Mass fractions:
 C  8.16064E-01  H  1.81489E-01  O  2.44670E-03
 Constitution:
 C3H8         9.70396E-01  C4H4_2       1.35135E-04  C2H4O2_ACETI 1.35135E-04
 C            1.35135E-04  C4H4_1       1.35135E-04  C2H4O1_OXIRA 1.35135E-04
 O2           1.35135E-04  C4H2_2       1.35135E-04  C2H4O1_ACETA 1.35135E-04
 O            1.35135E-04  C4H2_1       1.35135E-04  C2H4         1.35135E-04
 H2O2         1.35135E-04  C4H10_2      1.35135E-04  C2H3         1.35135E-04
 H2O1         1.35135E-04  C4H10_1      1.35135E-04  C2H2O1       1.35135E-04
 H2           1.35135E-04  C4H1         1.35135E-04  C2H2         1.35135E-04
 H1O2         1.35135E-04  C4           1.35135E-04  C2H1         1.35135E-04
 H1O1         1.35135E-04  C3O2         1.35135E-04  C2           1.35135E-04
 H            1.35135E-04  O3           1.35135E-04  C1O2         1.35135E-04
 C6H6O1       1.35135E-04  C3H6_2       1.35135E-04  C1O1         1.35135E-04
 C6H6         1.35135E-04  C3H6_1       1.35135E-04  C1H4O1       1.35135E-04
 C60          1.35135E-04  C3H6O1       1.35135E-04  C1H4         1.35135E-04
 C5           1.35135E-04  C3H4_2       1.35135E-04  C1H3O1_CH3O  1.35135E-04
 C4H8_6       1.35135E-04  C3H4_1       1.35135E-04  C1H3O1_CH2OH 1.35135E-04
 C4H8_5       1.35135E-04  C3H1         1.35135E-04  C1H3         1.35135E-04
 C4H8_4       1.35135E-04  C3           1.35135E-04  C1H2O2_TRANS 1.35135E-04
 C4H8_3       1.35135E-04  C2O1         1.35135E-04  C1H2O2_DIOXI 1.35135E-04
 C4H8_2       1.35135E-04  C2H6O2       1.35135E-04  C1H2O2_CIS   1.35135E-04
 C4H8_1       1.35135E-04  C2H6O1       1.35135E-04  C1H2O1       1.35135E-04
 C4H6_5       1.35135E-04  C2H6         1.35135E-04  C1H2         1.35135E-04
 C4H6_4       1.35135E-04  C2H5         1.35135E-04  C1H1O2       1.35135E-04
 C4H6_3       1.35135E-04  C2H4O3_124TR 1.35135E-04  C1H1O1       1.35135E-04
 C4H6_2       1.35135E-04  C2H4O3_123TR 1.35135E-04  C1H1         1.35135E-04
 C4H6_1       1.35135E-04  C2H4O2_DIOXE 1.35135E-04
POLY_3:Hit RETURN to continue
POLY_3: @@ We now have the initial amount of heat. Assuming an excess
POLY_3: @@ of oxygen we can calulate the temperature where the
POLY_3: @@ heat content whould be the same
POLY_3: sh h
   ... the command in full is SHOW_VALUE
 H=-99369.211
POLY_3: @@ H is just 11 times HM as there are 11 atoms in C3H8, save that value
POLY_3: @@ in a variable
POLY_3: enter var h298=h;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh h298
   ... the command in full is SHOW_VALUE
 H298=-99369.211
POLY_3: @@ If all carbon and hydrogen react with oxygen we need 7 oxygen atoms
POLY_3: @@ to form 3 moles C1O and 4 moles of H2O, add some oxygen in excess
POLY_3: s-c n(o)=9
   ... the command in full is SET_CONDITION
POLY_3: @@ Set the heat content as condition and remove the condition on t
POLY_3: s-c h=h298
   ... the command in full is SET_CONDITION
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /298.15/: none
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, N(O)=9, N(C)=3, N(H)=8, H=H298
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated            74 grid points in              0 s
   152 ITS,  CPU TIME USED    0 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB5

 Conditions:
 P=1E5, N(O)=9, N(C)=3, N(H)=8, H=H298
 DEGREES OF FREEDOM 0

 Temperature   3104.37 K (  2831.22 C),  Pressure  1.000000E+05
 Number of moles of components  2.00000E+01,  Mass in grams  1.88087E+02
 Total Gibbs energy -7.70908E+06,  Enthalpy -9.93692E+04,  Volume  2.20523E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
```

```
 C                        3.0000E+00  1.9158E-01 9.3493E-09 -4.7720E+05 SER
 H                        8.0000E+00  4.2869E-02 7.7490E-06 -3.0375E+05 SER
 O                        9.0000E+00  7.6555E-01 6.4120E-08 -4.2750E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 2.0000E+01, Mass 1.8809E+02, Volume fraction 1.0000E+00  Mass fractions:
 O  7.65554E-01  C  1.91576E-01  H  4.28695E-02
 Constitution:
 H2O1         3.17884E-01  C2H2         1.13693E-15  C3H6O1       1.00000E-30
 C1O1         2.27661E-01  C1H2O2_DIOXI 7.93238E-16  C3H6_1       1.00000E-30
 C1O2         1.23475E-01  C2H1         8.87885E-17  C3H6_2       1.00000E-30
 H1O1         8.79356E-02  C3O2         8.69739E-17  C3H8         1.00000E-30
 H2           7.64745E-02  C2           1.58189E-17  C4           1.00000E-30
 O2           6.60347E-02  C2H2O1       2.51164E-18  C4H1         1.00000E-30
 H            5.96672E-02  C2H3         2.70073E-19  C4H10_1      1.00000E-30
 O            4.08218E-02  C2H4O1_ACETA 1.21158E-20  C4H10_2      1.00000E-30
 H1O2         4.27603E-05  C2H4         1.11202E-20  C4H4_1       1.00000E-30
 H2O2         1.61649E-06  C2H4O2_ACETI 7.57727E-21  C4H8_4       1.00000E-30
 C1H1O1       9.35206E-07  C3H1         9.63256E-23  C4H8_5       1.00000E-30
 C1H1O2       6.81909E-07  C3           6.39018E-23  C4H4_2       1.00000E-30
 O3           3.02268E-08  C2H4O1_OXIRA 1.09569E-23  C4H6_1       1.00000E-30
 C1H2O2_CIS   1.60411E-08  C2H5         2.13496E-24  C4H6_2       1.00000E-30
 C1H2O2_TRANS 8.96990E-09  C2H6         2.28920E-26  C4H6_3       1.00000E-30
 C1H2O1       7.23694E-09  C2H6O1       6.22800E-27  C4H6_4       1.00000E-30
 C            5.44356E-11  C2H6O2       8.36793E-28  C4H8_6       1.00000E-30
 C1H1         5.72382E-12  C3H4_2       5.27771E-28  C4H6_5       1.00000E-30
 C1H2         2.82162E-12  C3H4_1       2.83571E-28  C5           1.00000E-30
 C1H3         2.07810E-12  C2H4O2_DIOXE 1.26547E-29  C60          1.00000E-30
 C2O1         1.16914E-12  C2H4O3_124TR 2.44217E-30  C4H8_1       1.00000E-30
 C1H3O1_CH2OH 8.91882E-13  C4H2_1       2.35081E-30  C6H6         1.00000E-30
 C1H4         1.78630E-13  C4H2_2       2.34436E-30  C6H6O1       1.00000E-30
 C1H3O1_CH3O  1.92065E-14  C4H8_3       1.00000E-30  C4H8_2       1.00000E-30
 C1H4O1       9.71550E-15  C2H4O3_123TR 1.00000E-30
POLY_3: @@ The adiabatic temperature is
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=3104.3748
POLY_3:Hit RETURN to continue
POLY_3: @@ Now calculate how the adiabatic temperature varies with
POLY_3: @@ the amount of oxygen
POLY_3: s-a-v 1 n(o) 5 10
   ... the command in full is SET_AXIS_VARIABLE
Increment /.125/:
POLY_3: save tcex22 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value     9.00000
...OK

 Phase Region from     9.00000      for:
     GAS
 Global test at  1.00000E+01 .... OK
 Terminating at   10.00000
 Calculated    11 equilibria

 Phase Region from     9.00000      for:
     GAS
 Global test at  8.00000E+00 .... OK
 Global test at  6.75000E+00 .... OK
 Global test at  5.50000E+00 .... OK
 Terminating at    5.00000
 Calculated    35 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex22\tcex
 22.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST:
POST: s-d-a x n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

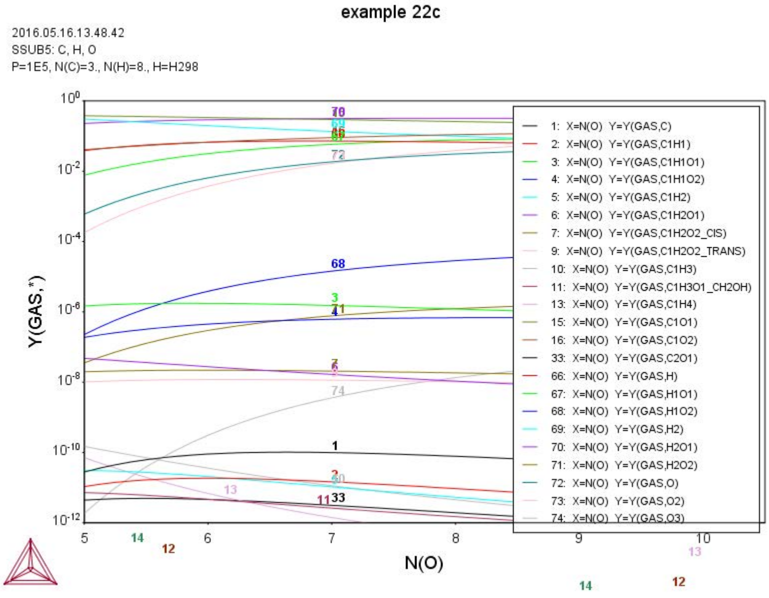


```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the gas constitition changes
```

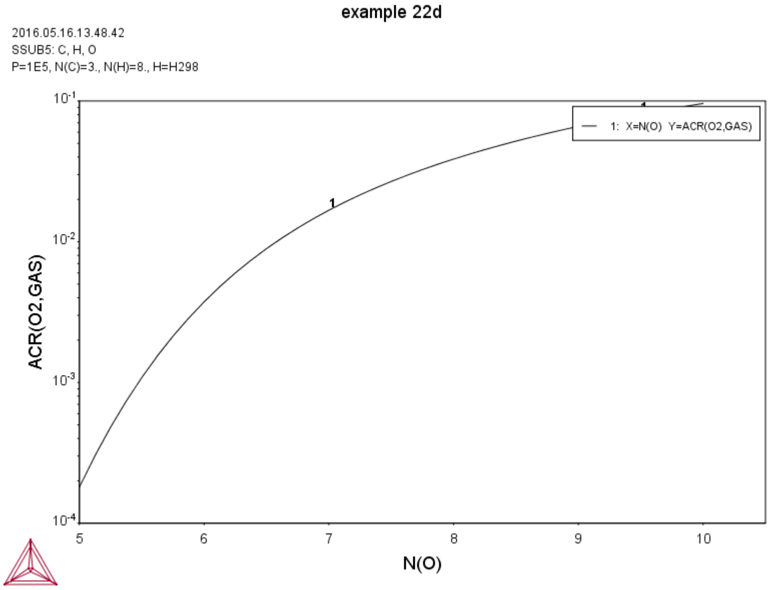
```
POST: s-d-a y y(gas,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 22b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



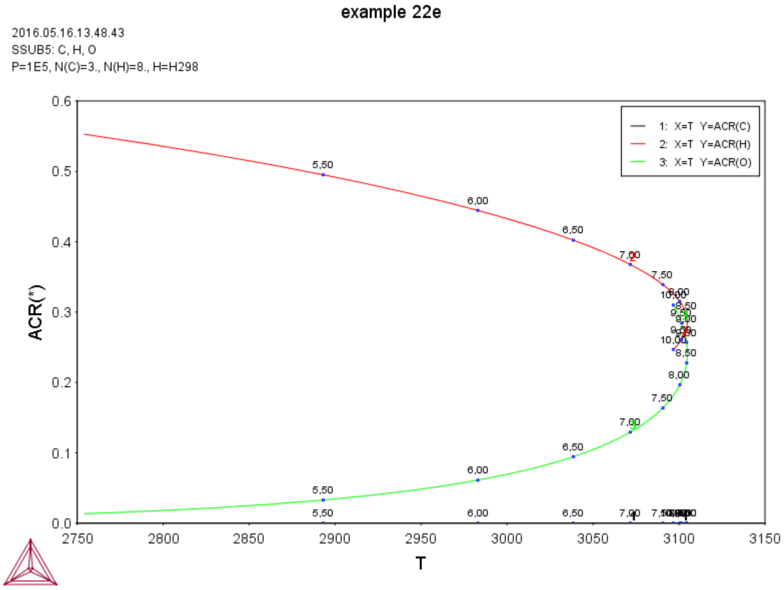
```
POST:
POST:Hit RETURN to continue
POST: @@ Add labels and logarithmic fraction scale
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-s y n 1e-12 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 22c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the oxygen partial pressure changes
POST: s-d-a y acr(o2,gas)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the activies of the components change with temperature
POST: @@ Note that the oxygen content changes also ...
POST: @@ We must set reference states
POST: set-ref-state o gas * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state h gas * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state c c_s * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: s-d-a x t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty y lin
   ... the command in full is SET_AXIS_TYPE
POST: s-d-a z n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 5 10
   ... the command in full is SET_SCALING_STATUS
POST: s-d-a y acr(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 22e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex23

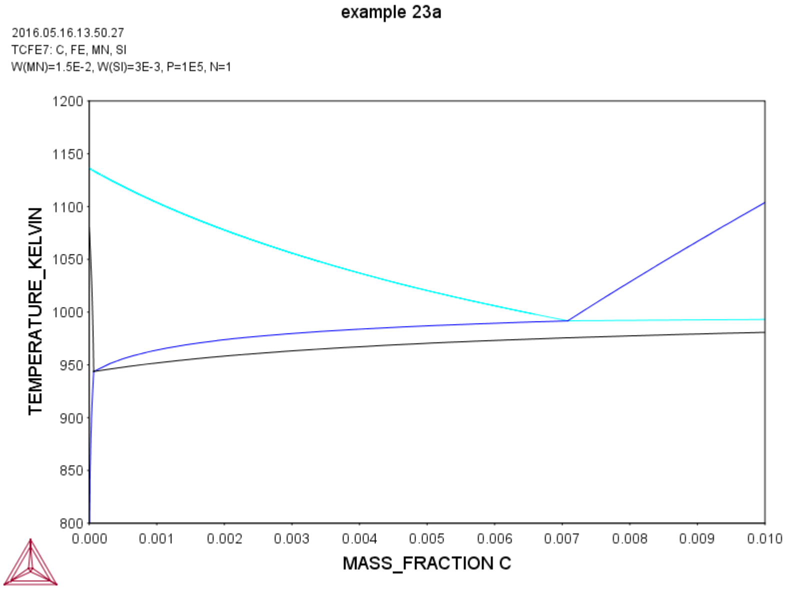
```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex23\tcex23.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of T-zero and paraequilibria in a low alloyed steel
SYS: @@
SYS: set-log ex23,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ Define the material
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: mn 1.5
2nd alloying element: si .3
Next alloying element: c .3
Next alloying element:
Temperature (C) /1000/: 700
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M5C2                     KSI_CARBIDE
 A1_KAPPA                 KAPPA                    FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14          M3SI
 G_PHASE                  CR3SI                    FE2SI
 MSI                      M5SI3                    AL4C3
 FE8SI2C                  SIC

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

 ........................................................

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M5C2                     KSI_CARBIDE
 A1_KAPPA                 KAPPA                    FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14          M3SI
 G_PHASE                  CR3SI                    FE2SI
 MSI                      M5SI3                    AL4C3
 FE8SI2C                  SIC

 ........................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'J. Grobner, H.L. Lukas and F. Aldinger, Calphad, 20 (1996), 247-254; Si-C
      and Al-Si-C'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe
      -Si-C'
  'J.E. Tibballs, SI Norway (1991) Rep. 890221-5; Mn-Si'
  'P. Franke, estimated parameter within SGTE, 2008; Fe-Mn-C'
  'B. Sundman, 1999, revision of the liquid Fe-Si-C description'
  'NPL, unpublished work (1989); C-Mn-Si'
  'A. Forsberg and J. Agren, J. Phase Equil., 14 (1993), 354-363; Fe-Mn-Si'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
```

```
   'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
       1989); C-FE-MN'
   'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
   'Unassessed parameter'
   'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
   'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
       data for intermetallic phases. Metals park, Ohio. American Society for
       Metals; Molar volumes'
   'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
       C-CR-FE'
   'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
   'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
   'Thermo-Calc Software (2008): Volume data updated for TCFE6 database (TCFE
       v6, April, 2008).'
   'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C-FE-MO'
   'D. Connetable, J. Lacaze, P. Maugis and B. Sundman; Calphad, Vol. 32
       (2008), pp. 361-370; Al-C-Fe'
   'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
   'Estimated parameter for solubility of C in Fe4N, 1999'
   'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
        441-448; Fe-Ti'
   'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
   'N. Saunders, COST 507 Report (1998); Mn-Ti'
   'B.-J. Lee, KRISS, unpublished research, during 1993-1995'
   'I. Ansara, unpublished work (1991); Cr-Si'
   'A. Markstrom, Thermo-Calc software AB, 2011'
  -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         16035 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    973.15 K (   700.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50671E+01
 Total Gibbs energy -4.16088E+04,  Enthalpy  2.38836E+04,  Volume  7.24185E-06

 Component               Moles      W-Fraction  Activity   Potential  Ref.stat
 C                       1.3754E-02  3.0000E-03 2.2665E-01 -1.2010E+04 SER
 FE                      9.6533E-01  9.7900E-01 6.6031E-03 -4.0620E+04 SER
 MN                      1.5035E-02  1.5000E-02 6.5723E-05 -7.7919E+04 SER
 SI                      5.8820E-03  3.0000E-03 2.1018E-10 -1.8030E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.4142E-01, Mass 4.1252E+01, Volume fraction 7.4788E-01  Mass fractions:
 FE  9.87818E-01  MN  8.85142E-03  SI  3.22070E-03  C   1.10187E-04

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 2.5248E-01, Mass 1.3742E+01, Volume fraction 2.4758E-01  Mass fractions:
 FE  9.57752E-01  MN  3.35378E-02  C   6.35700E-03  SI  2.35347E-03

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 6.1027E-03, Mass 7.3300E-02, Volume fraction 4.5452E-03  Mass fractions:
 C   1.00000E+00  SI  0.00000E+00  MN  0.00000E+00  FE  0.00000E+00
POLY_3: @@ Suspend some phases that normally never appear
POLY_3: ch-st p gra m5c2=sus
   ... the command in full is CHANGE_STATUS
POLY_3:Hit RETURN to continue
POLY_3: @@ Set axis for T-w(c) phase diagram
POLY_3: s-a-v 1 w(c)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .01
Increment /2.5E-04/: 2.5E-04
POLY_3: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 800
Max value /1/: 1200
Increment /10/: 30
POLY_3: save tcex23a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
```

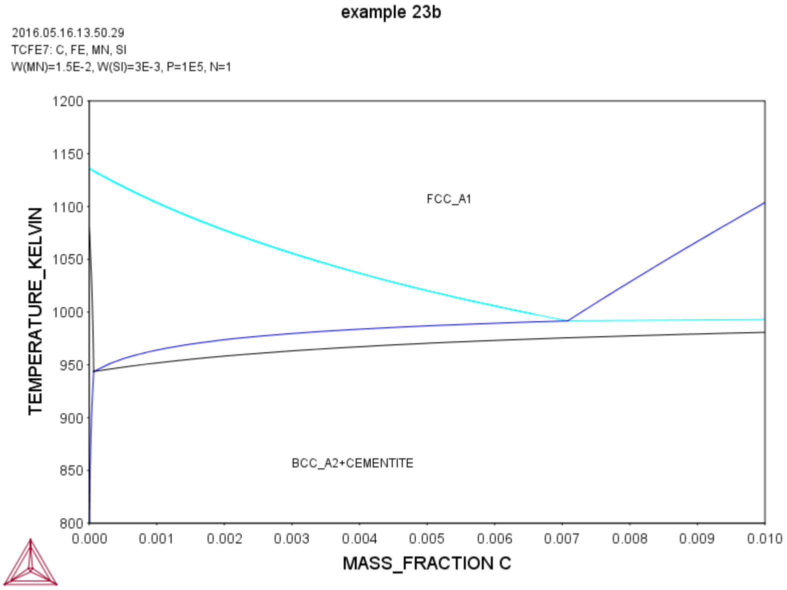
```
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24

Phase region boundary   1 at:   2.500E-04  9.455E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                      3  equilibria

Phase region boundary   2 at:   6.694E-05  9.437E+02
    BCC_A2
 ** CEMENTITE
 ** FCC_A1

Phase region boundary   3 at:   6.694E-05  9.437E+02
    BCC_A2
 ** FCC_A1
Calculated                     18  equilibria

Phase region boundary   4 at:   6.694E-05  9.437E+02
    BCC_A2
 ** CEMENTITE
Calculated..                     10  equilibria
Terminating at axis limit.

Phase region boundary   5 at:   6.694E-05  9.437E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     31  equilibria

Phase region boundary   6 at:   7.080E-03  9.917E+02
 ** BCC_A2
 ** CEMENTITE
    FCC_A1

Phase region boundary   7 at:   7.080E-03  9.917E+02
 ** CEMENTITE
    FCC_A1
Calculated..                     17  equilibria
Terminating at axis limit.

Phase region boundary   8 at:   7.080E-03  9.917E+02
 ** BCC_A2
    FCC_A1
Calculated                     43  equilibria

Phase region boundary   9 at:   7.080E-03  9.917E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1
Calculated..                     13  equilibria
Terminating at axis limit.

Phase region boundary  10 at:   6.694E-05  9.437E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     42  equilibria
Terminating at axis limit.

Phase region boundary  11 at:   2.500E-04  9.455E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     41  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  12 at:   3.417E-03  9.650E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  13 at:   3.417E-03  9.650E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     28  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  14 at:   6.583E-03  9.745E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     28  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   6.583E-03  9.745E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     16  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   6.157E-06  8.100E+02
    BCC_A2
 ** CEMENTITE
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  17 at:   6.157E-06  8.100E+02
```

```
    BCC_A2
 ** CEMENTITE
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   9.750E-03  9.804E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     40  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   9.750E-03  9.804E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     3  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   6.040E-05  9.367E+02
    BCC_A2
 ** CEMENTITE
Calculated..                    10  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  21 at:   6.040E-05  9.367E+02
    BCC_A2
 ** CEMENTITE
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   2.642E-03  1.063E+03
 ** BCC_A2
    FCC_A1
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   2.642E-03  1.063E+03
 ** BCC_A2
    FCC_A1
Calculated                     23  equilibria

Phase region boundary  24 at:   8.904E-03  1.063E+03
 ** CEMENTITE
    FCC_A1
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   8.904E-03  1.063E+03
 ** CEMENTITE
    FCC_A1
Calculated..                     7  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  26 at:   2.500E-04  1.127E+03
 ** BCC_A2
    FCC_A1
Calculated                     22  equilibria

Phase region boundary  27 at:   2.500E-04  1.127E+03
 ** BCC_A2
    FCC_A1
Calculated.                     29  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   3.417E-03  1.048E+03
 ** BCC_A2
    FCC_A1
Calculated                     26  equilibria

Phase region boundary  29 at:   3.417E-03  1.048E+03
 ** BCC_A2
    FCC_A1
Calculated.                     16  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   6.583E-03  9.981E+02
 ** BCC_A2
    FCC_A1
Calculated                     38  equilibria

Phase region boundary  31 at:   6.583E-03  9.981E+02
 ** BCC_A2
    FCC_A1
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   9.750E-03  1.095E+03
 ** CEMENTITE
    FCC_A1
Calculated.                     12  equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   9.750E-03  1.095E+03
 ** CEMENTITE
    FCC_A1
Calculated..                     3  equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex23\tcex
23a.POLY3
CPU time for mapping                       8  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST: set-title example 23a
POST: plot
```

```
   ... the command in full is PLOT_DIAGRAM
```

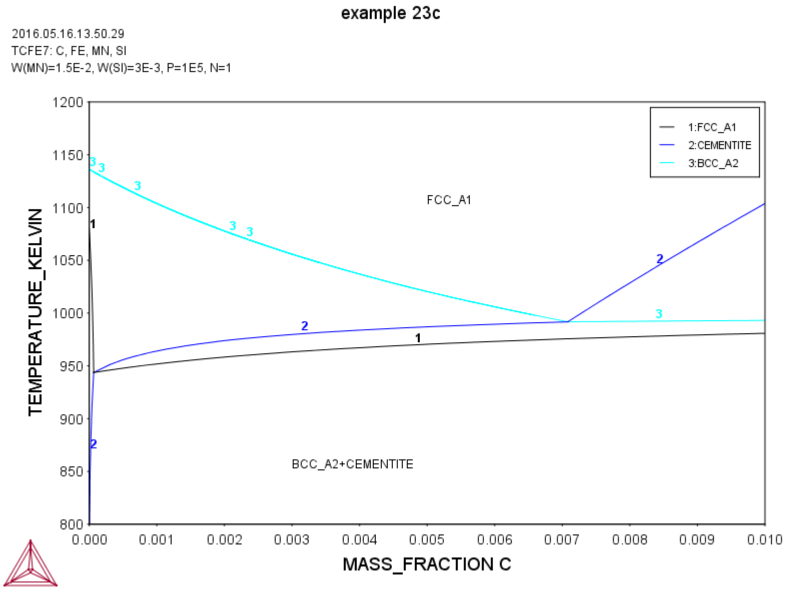


```
POST:
POST:Hit RETURN to continue
POST: @@ Add labels
POST: add
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .005
Give Y coordinate in axis units: 1100
Automatic phase labels? /Y/: Y
 Automatic labelling not always possible
 Using global minimization procedure
Calculated         15897 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       1 s, total time      1  s
 Stable phases are: FCC_A1
Text size: /.36/: .34
POST: add
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .003
Give Y coordinate in axis units: 850
Automatic phase labels? /Y/: Y
 Automatic labelling not always possible
 Using global minimization procedure
Calculated         15897 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: BCC_A2+CEMENTITE
Text size: /.36/: .34
POST: set-title example 23b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



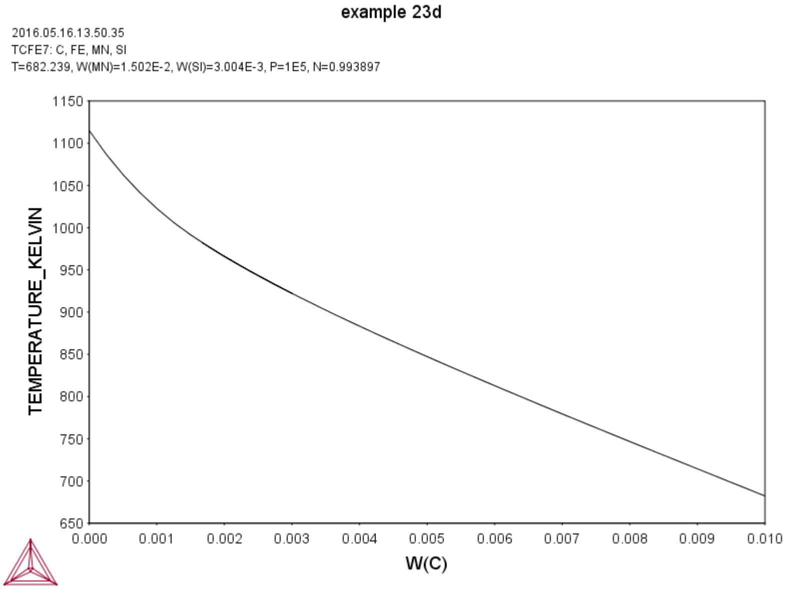
```
POST:
POST:Hit RETURN to continue
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: ?
 THE OPTIONS MEANS:
 A      LIST STABLE PHASES ALONG LINE
 B      AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
 C      LIST AXIS QUANTITIES
 D      AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
 E      AS B WITH CHANGING COLORS
 F      AS D WITH CHANGING COLORS
 N      NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: e
POST: set-title example 23c
POST:
```

```
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

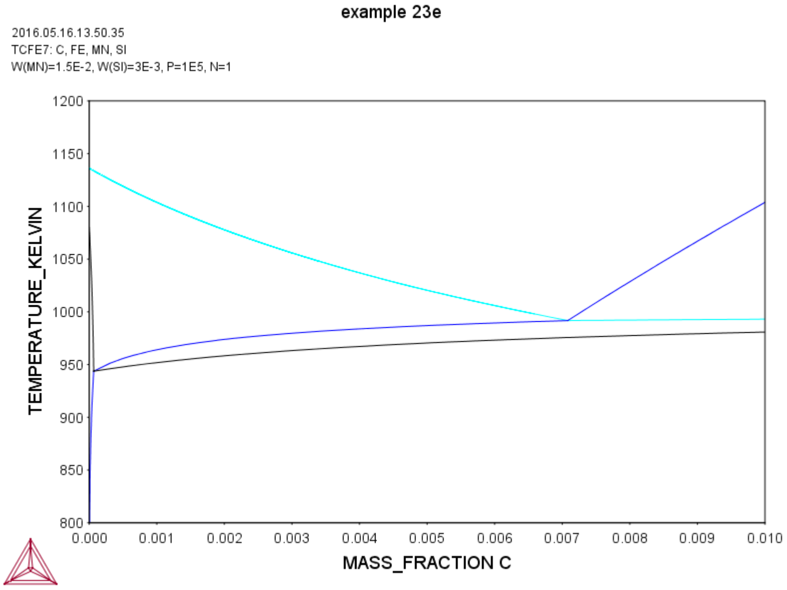


```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: @@ Now calculate the T-zero temperature for the steel
POLY_3: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY_3: advanced-options
Which option? /STEP_AND_MAP/: ?
 EQUILIBRIUM_CALCUL        NEW_COMPOSITION_SET       SHOW_FOR_T=
 GLOBAL_MINIMIZATION       OUTPUT_FILE_FOR_SHOW      STABILITY_CHECK
 IGNORE_COMPOSI_SET_ORDER PARAEQUILIBRIUM           STEP_AND_MAP
 LIST_PHASE_ADDITION       PHASE_ADDITION            T-ZERO TEMPERATURE
 MAJOR_CONSTITUENTS        PRESENT_PHASE             TOGGLE_ALTERNATE_MODE
Which option? /STEP_AND_MAP/: t-z

This command calculates the temperature when two phases have the same Gibbs
energy.  You must calculate an equilibrium at an estimated temperature first.
Name of first phase: fcc
Name of second phase: bcc

 The T0 temperature is  922.21 K
 Note: LIST-EQUILIBRIUM is not relevant
POLY_3:Hit RETURN to continue
POLY_3: @@ Calculate the T-zero line, remove the T-axis
POLY_3: l-ax
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(C)                   Min: 0         Max: 1E-2      Inc: 2.5E-4
  Axis No 2: T                      Min: 800       Max: 1200      Inc: 30
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex23b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: ?
 The following options are available:
 NORMAL              Stepping with given conditions
 INITIAL_EQUILIBRIA An initial equilibrium stored at every step
 EVALUATE            Specified variables evaluated after each step
 SEPARATE_PHASES     Each phase calculated separately
 T-ZERO              T0 line calculation
 PARAEQUILIBRIUM     Paraequilibrium diagram
 MIXED_SCHEIL        Scheil with fast diffusing elements
 ONE_PHASE_AT_TIME  One phase at a time
Option? /NORMAL/: t-z
Name of first phase: fcc
Name of second phase: bcc

 Phase Region from   0.300000E-02 for:
     BCC_A2
     FCC_A1
   3.000000E-03         922.21
   2.750000E-03         932.54
   2.500000E-03         943.23
   2.250000E-03         954.34
   2.000000E-03         965.98
   1.750000E-03         978.31
   1.500000E-03         991.57
   1.250000E-03        1006.14
   1.000000E-03        1022.76
   7.500000E-04        1041.59
   5.000000E-04        1062.86
   2.500000E-04        1087.12
   2.500000E-10        1115.11

 Phase Region from   0.167112E-02 for:
     BCC_A2
     FCC_A1
   1.671124E-03         982.32
   1.921124E-03         969.73
   2.171124E-03         957.89
   2.421124E-03         946.63
   2.671124E-03         935.82
   2.921124E-03         925.38
   3.171124E-03         915.26
   3.421124E-03         905.40
   3.671124E-03         895.77
   3.921124E-03         886.33
```

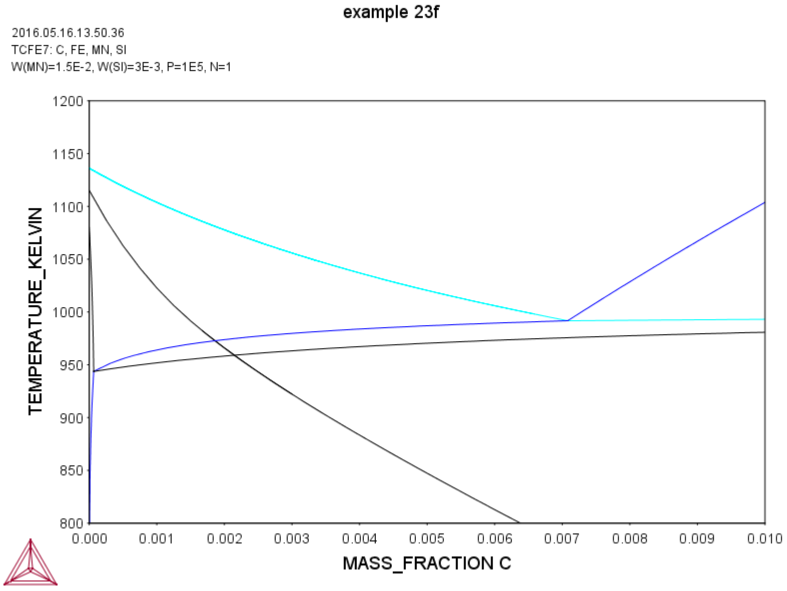
```
   4.171124E-03         877.06
   4.421124E-03         867.93
   4.671124E-03         858.95
   4.921124E-03         850.07
   5.171124E-03         841.30
   5.421124E-03         832.63
   5.671124E-03         824.03
   5.921124E-03         815.51
   6.171124E-03         807.06
   6.421124E-03         798.67
   6.671124E-03         790.33
   6.921124E-03         782.04
   7.171124E-03         773.79
   7.421124E-03         765.58
   7.671124E-03         757.40
   7.921124E-03         749.26
   8.171124E-03         741.14
   8.421124E-03         733.04
   8.671124E-03         724.96
   8.921124E-03         716.90
   9.171124E-03         708.85
   9.421124E-03         700.82
   9.671124E-03         692.79
   9.921124E-03         684.77
   1.000000E-02         682.24
 *** Buffer savend on file
 c:\jenkins\WORKSP~1\THERMO~1\examples\tcex23\TCEX23~2.POL
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST:
POST: set-title example 23d
POST: s-d-a x w(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ write the line on a data file
POST: make tcex23b y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: ba
   ... the command in full is BACK
POLY_3: @@ plot together with phase diagram
POLY_3: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST: set-title example 23e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

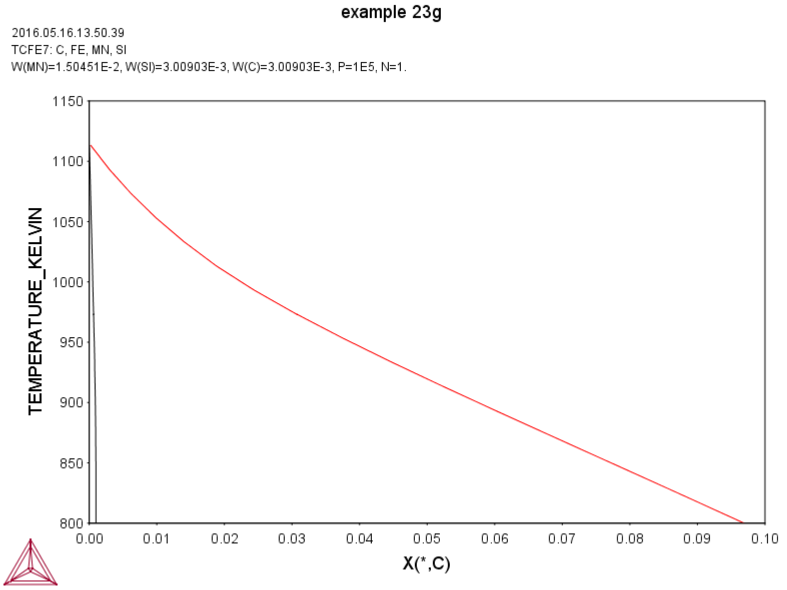


```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23b
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23f
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

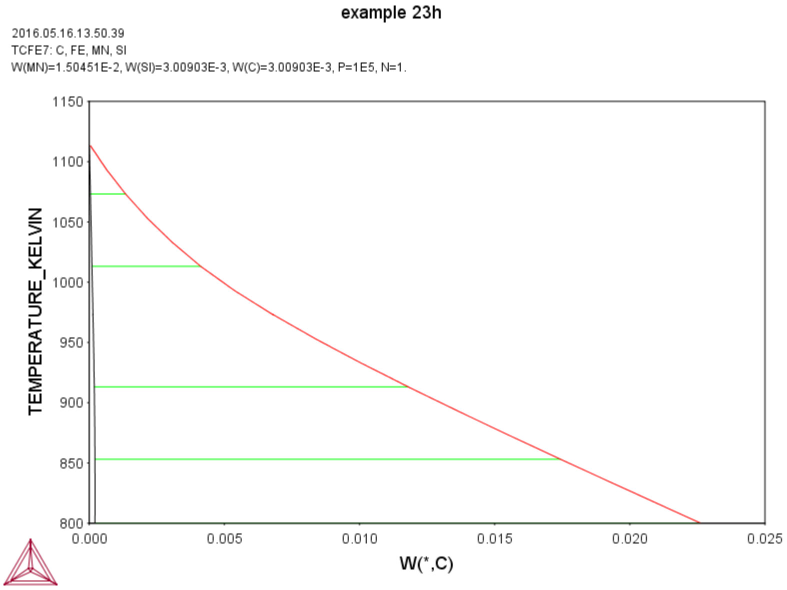


```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: @@ Now calculate the para-equilibrium for the steel
POLY_3: @@ At paraequilibrium only C is mobile, the other alloying elements have
POLY_3: @@ the same compositions in both phases
POLY_3: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         15897 grid points in              0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    973.15 K (   700.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50671E+01
 Total Gibbs energy -4.16068E+04,  Enthalpy  2.38034E+04,  Volume  7.22424E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        1.3754E-02  3.0000E-03 2.3682E-01 -1.1655E+04 SER
 FE                       9.6533E-01  9.7900E-01 6.6051E-03 -4.0617E+04 SER
 MN                       1.5035E-02  1.5000E-02 6.2466E-05 -7.8331E+04 SER
 SI                       5.8820E-03  3.0000E-03 2.1440E-10 -1.8014E+05 SER

 BCC_A2                       Status ENTERED     Driving force  0.0000E+00
 Moles 7.6441E-01, Mass 4.2529E+01, Volume fraction 7.7288E-01  Mass fractions:
 FE  9.88221E-01  MN  8.40073E-03  SI  3.26359E-03  C   1.14706E-04

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
```

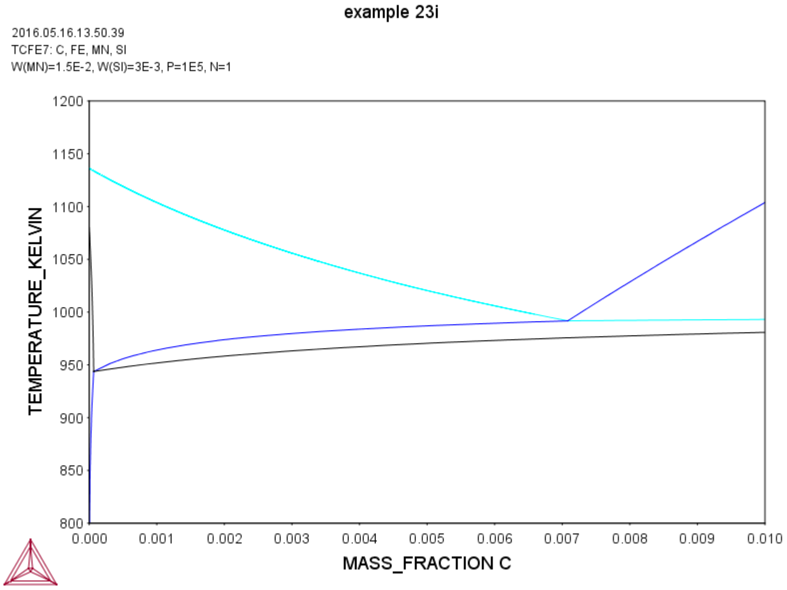
```
 Moles 2.0669E-01, Mass 1.1242E+01, Volume fraction 2.0306E-01  Mass fractions:
 FE  9.59011E-01  MN  3.21007E-02  C   6.54001E-03  SI  2.34865E-03

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.8906E-02, Mass 1.2957E+00, Volume fraction 2.4065E-02  Mass fractions:
 FE  8.49786E-01  MN  8.32277E-02  C   6.69864E-02  SI  4.69914E-13
POLY_3: advance para
   ... the command in full is ADVANCED_OPTIONS

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
 NP(FCC) =   0.4280 with U-fractions C  =  3.17220E-02
 NP(BCC) =   0.5720 with U-fractions C  =  6.47538E-04
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3:
POLY_3: @@ Now calculate the para-equilibrium for the steel at varying temperatures
POLY_3: s-a-v 1 t 800 1200 20
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex23c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step para
   ... the command in full is STEP_WITH_OPTIONS

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    973.150     for:
     BCC_A2
     FCC_A1
   9.731500E+02    0.428    0.572   3.172200E-02   6.475377E-04  -1.290452E+00
   9.531500E+02    0.345    0.655   3.908052E-02   7.297760E-04  -8.659516E-01
   9.331500E+02    0.285    0.715   4.699458E-02   8.039957E-04  -4.522834E-01
   9.131500E+02    0.240    0.760   5.535054E-02   8.679372E-04  -4.631426E-02
   8.931500E+02    0.206    0.794   6.405501E-02   9.201210E-04   3.549783E-01
   8.731500E+02    0.180    0.820   7.303132E-02   9.596491E-04   7.543208E-01
   8.531500E+02    0.160    0.840   8.221743E-02   9.860983E-04   1.154160E+00
   8.331500E+02    0.143    0.857   9.156332E-02   9.994314E-04   1.556708E+00
   8.131500E+02    0.129    0.871   1.010286E-01   9.999336E-04   1.963997E+00
   8.000000E+02    0.122    0.878   1.073012E-01   9.935324E-04   2.235299E+00

 Phase Region from    973.150     for:
     BCC_A2
     FCC_A1
   9.731500E+02    0.429    0.571   3.168117E-02   6.465368E-04  -1.292139E+00
   9.931500E+02    0.547    0.453   2.501532E-02   5.595693E-04  -1.730355E+00
   1.013150E+03    0.720    0.280   1.919684E-02   4.725723E-04  -2.182535E+00
   1.033150E+03    0.977    0.023   1.426175E-02   3.879729E-04  -2.653059E+00
   1.053150E+03    1.411   -0.411   9.973814E-03   3.003908E-04  -3.172815E+00
   1.073150E+03    2.275   -1.275   6.247344E-03   2.085287E-04  -3.792875E+00
   1.093150E+03    4.762   -3.762   3.016699E-03   1.116447E-04  -4.664306E+00
   1.113150E+03   64.105  -63.105   2.267080E-04   9.302453E-06  -7.388093E+00
 *** Buffer savend on file
 c:\jenkins\WORKSP~1\THERMO~1\examples\tcex23\TCEX23~3.POL

 *** ERROR     7 IN NS01AD
 *** Numerical error
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: set-title example 23g
POST: s-d-a x x(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



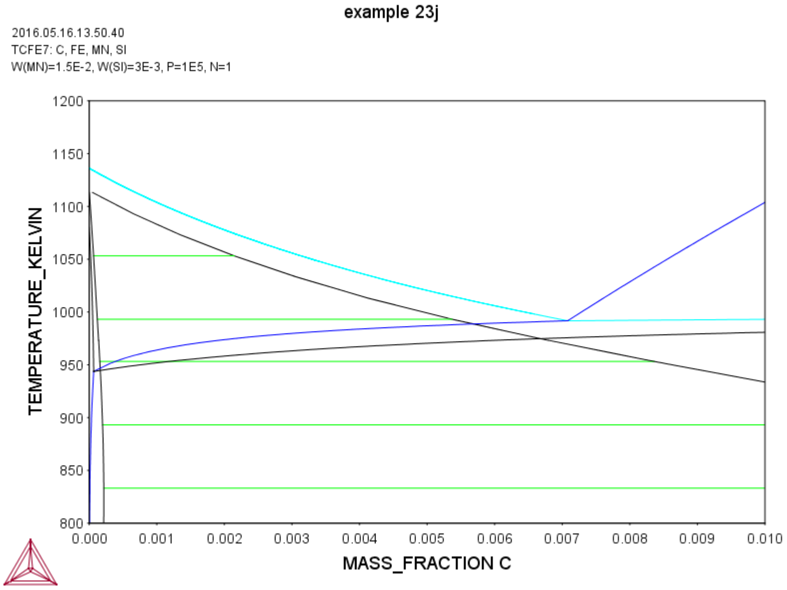
```
POST:
POST:Hit RETURN to continue
POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: s-t-s 3
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 23h
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



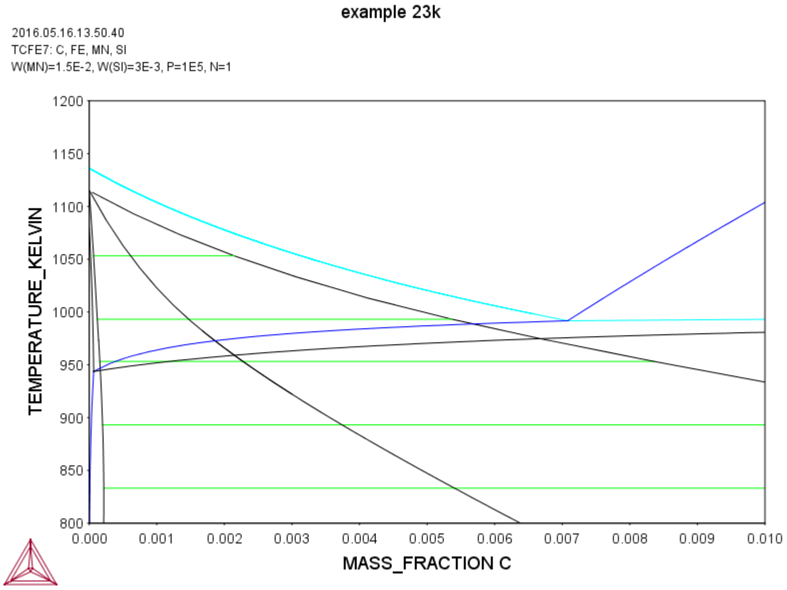
```
POST:
POST:Hit RETURN to continue
POST: make tcex23c y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: ba
   ... the command in full is BACK
POLY_3: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: set-title example 23i
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23c
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23j
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23b.exp tcex23c.exp 0; 1; 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: set-title example 23k
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

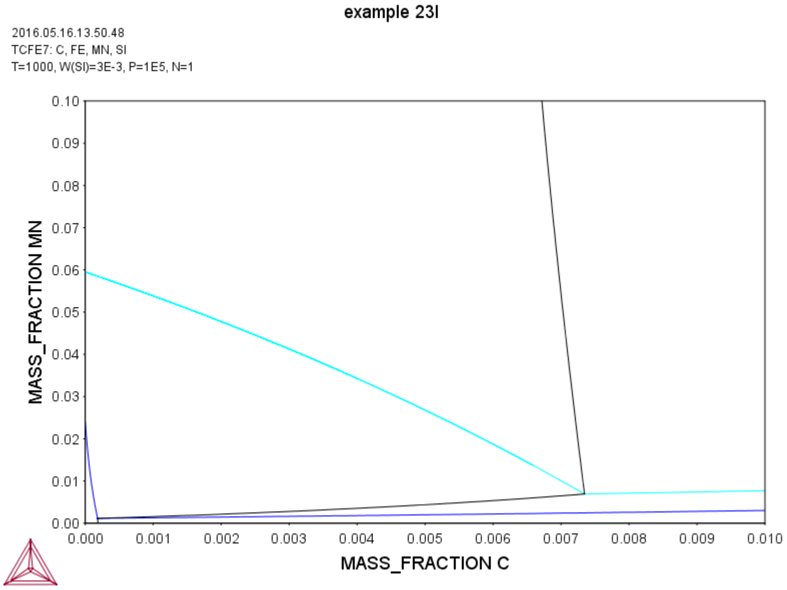


```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: @@ Now calculate both a normal and para-equilibrium for the steel at 1000 K
POLY_3: @@ Note that a para equilibrium does not always exist for the given conditions
POLY_3: @@ The calculated results are the amounts of the two phases.
POLY_3: @@ This indicates how much of the phases that can be tranformed
POLY_3: @@ at para-equilibrium conditions.
POLY_3: @@ The carbon content of the phases are also listed,
POLY_3: @@ the other alloying elements have the same fractions in both phases
POLY_3: read tcex23a.POLY3
   ... the command in full is READ_WORKSPACES
POLY_3: s-c T=1000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         15897 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1000, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50671E+01
 Total Gibbs energy -4.34548E+04,  Enthalpy  2.63172E+04,  Volume  7.20607E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        1.3754E-02  3.0000E-03 1.6744E-01 -1.4859E+04 SER
 FE                       9.6533E-01  9.7900E-01 6.1057E-03 -4.2392E+04 SER
 MN                       1.5035E-02  1.5000E-02 4.1161E-05 -8.3960E+04 SER
 SI                       5.8820E-03  3.0000E-03 3.4194E-10 -1.8123E+05 SER

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
 Moles 5.3820E-01, Mass 2.9381E+01, Volume fraction 5.3141E-01  Mass fractions:
 FE  9.69754E-01  MN  2.22121E-02  C    5.51915E-03  SI  2.51464E-03

 BCC_A2                       Status ENTERED     Driving force  0.0000E+00
 Moles 4.6180E-01, Mass 2.5686E+01, Volume fraction 4.6859E-01  Mass fractions:
 FE  9.89576E-01  MN  6.75038E-03  SI  3.55518E-03  C   1.18465E-04
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
 NP(FCC) =    0.5982 with U-fractions C   =  2.29562E-02
 NP(BCC) =    0.4018 with U-fractions C   =  5.30475E-04
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ Now calculate an isothermal phase diagram at 1000 K
POLY_3: s-a-v 2 w(mn) 0 .1,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:Hit RETURN to continue
POLY_3: save tcex23d y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
```

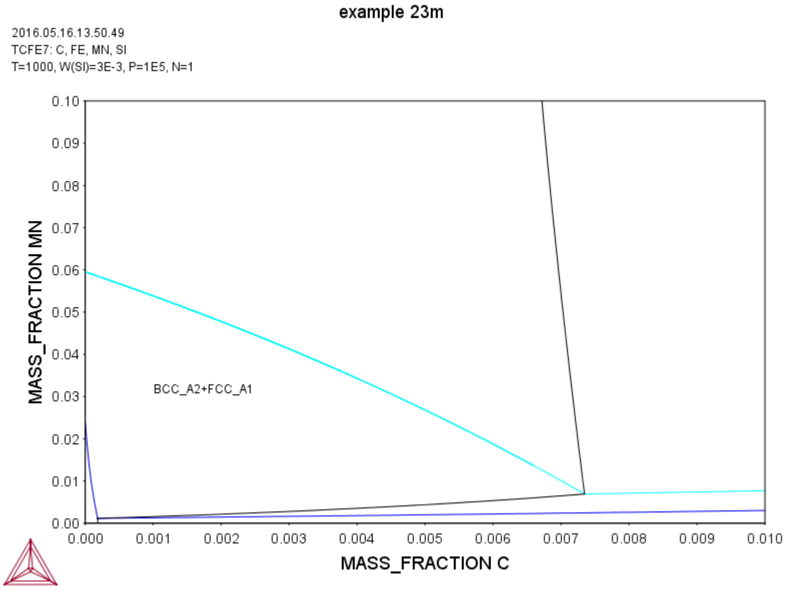
```
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
 Generating start point  31
 Generating start point  32

 Phase region boundary   1 at:   2.585E-03  2.500E-03
     BCC_A2
  ** CEMENTITE
     FCC_A1
 Calculated.                     11  equilibria

 Phase region boundary   2 at:   1.821E-04  1.138E-03
     BCC_A2
  ** CEMENTITE
  ** FCC_A1

 Phase region boundary   3 at:   1.821E-04  1.138E-03
     BCC_A2
  ** CEMENTITE
 Calculated                     14  equilibria

 Phase region boundary   4 at:   1.821E-04  1.138E-03
     BCC_A2
  ** FCC_A1
 Calculated                     24  equilibria

 Phase region boundary   5 at:   1.821E-04  1.138E-03
     BCC_A2
     CEMENTITE
  ** FCC_A1
 Calculated..                     41  equilibria
 Terminating at axis limit.

 Phase region boundary   6 at:   1.821E-04  1.138E-03
     BCC_A2
  ** CEMENTITE
     FCC_A1
 Calculated.                     30  equilibria

 Phase region boundary   7 at:   7.345E-03  6.913E-03
  ** BCC_A2
  ** CEMENTITE
     FCC_A1

 Phase region boundary   8 at:   7.345E-03  6.913E-03
  ** CEMENTITE
     FCC_A1
 Calculated..                     39  equilibria
 Terminating at axis limit.

 Phase region boundary   9 at:   7.345E-03  6.913E-03
  ** BCC_A2
     FCC_A1
 Calculated                     40  equilibria

 Phase region boundary  10 at:   7.345E-03  6.913E-03
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated..                     13  equilibria
 Terminating at axis limit.

 Phase region boundary  11 at:   2.585E-03  2.500E-03
     BCC_A2
  ** CEMENTITE
     FCC_A1
 Calculated.                     21  equilibria
 Terminating at known equilibrium

 Phase region boundary  12 at:   2.500E-04  5.813E-02
  ** BCC_A2
     FCC_A1
 Calculated                     22  equilibria

 Phase region boundary  13 at:   2.500E-04  5.813E-02
  ** BCC_A2
     FCC_A1
 Calculated.                     30  equilibria
```

```
Terminating at known equilibrium

Phase region boundary  14 at:   3.417E-03  3.078E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   3.417E-03  3.078E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     17  equilibria
Terminating at known equilibrium

Phase region boundary  16 at:   6.583E-03  5.991E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     27  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   6.583E-03  5.991E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                      5  equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   7.601E-03  2.500E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     31  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.601E-03  2.500E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     11  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   9.750E-03  2.959E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     40  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   9.750E-03  2.959E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                      3  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   4.016E-03  3.417E-02
 ** BCC_A2
    FCC_A1
Calculated.                     22  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   4.016E-03  3.417E-02
 ** BCC_A2
    FCC_A1
Calculated                     33  equilibria

Phase region boundary  24 at:   7.141E-03  3.417E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     12  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   7.141E-03  3.417E-02
 ** CEMENTITE
    FCC_A1
Calculated..                     28  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  26 at:   6.924E-03  6.583E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     25  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   6.924E-03  6.583E-02
 ** CEMENTITE
    FCC_A1
Calculated..                     15  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:   6.924E-03  6.583E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     25  equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   6.924E-03  6.583E-02
 ** CEMENTITE
    FCC_A1
Calculated..                     15  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  30 at:   6.732E-03  9.750E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     38  equilibria
Terminating at known equilibrium
```

```
 Phase region boundary  31 at:   6.732E-03  9.750E-02
  ** CEMENTITE
     FCC_A1
 Calculated..                      3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  32 at:   2.500E-04  5.813E-02
  ** BCC_A2
     FCC_A1
 Calculated                      4  equilibria

 Phase region boundary  33 at:   2.500E-04  5.813E-02
  ** BCC_A2
     FCC_A1
 Calculated.                     30  equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   3.417E-03  3.841E-02
  ** BCC_A2
     FCC_A1
 Calculated                     26  equilibria

 Phase region boundary  35 at:   3.417E-03  3.841E-02
  ** BCC_A2
     FCC_A1
 Calculated.                     17  equilibria
 Terminating at known equilibrium

 Phase region boundary  36 at:   6.583E-03  1.374E-02
  ** BCC_A2
     FCC_A1
 Calculated                     38  equilibria

 Phase region boundary  37 at:   6.583E-03  1.374E-02
  ** BCC_A2
     FCC_A1
 Calculated.                      5  equilibria
 Terminating at known equilibrium

 Phase region boundary  38 at:   6.732E-03  9.750E-02
  ** CEMENTITE
     FCC_A1
 Calculated.                     38  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.732E-03  9.750E-02
  ** CEMENTITE
     FCC_A1
 Calculated..                      3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  40 at:   9.750E-03  7.619E-03
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated.                     11  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.750E-03  7.619E-03
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated..                      3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex23\tcex
 23d.POLY3
 CPU time for mapping                      5  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: set-title example 23l
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

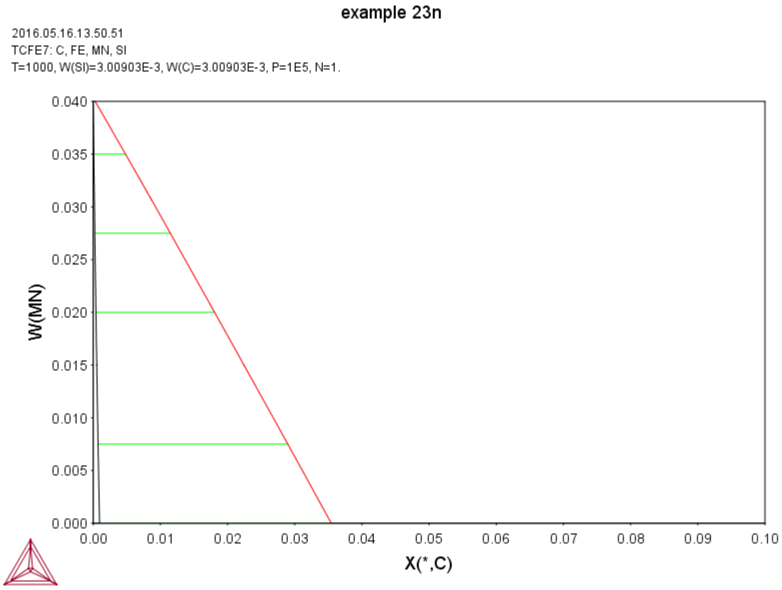


```
POST:
POST:Hit RETURN to continue
POST: add .001 .03,,,,
   ... the command in full is ADD_LABEL_TEXT
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: BCC_A2+FCC_A1
POST: set-title example 23m
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

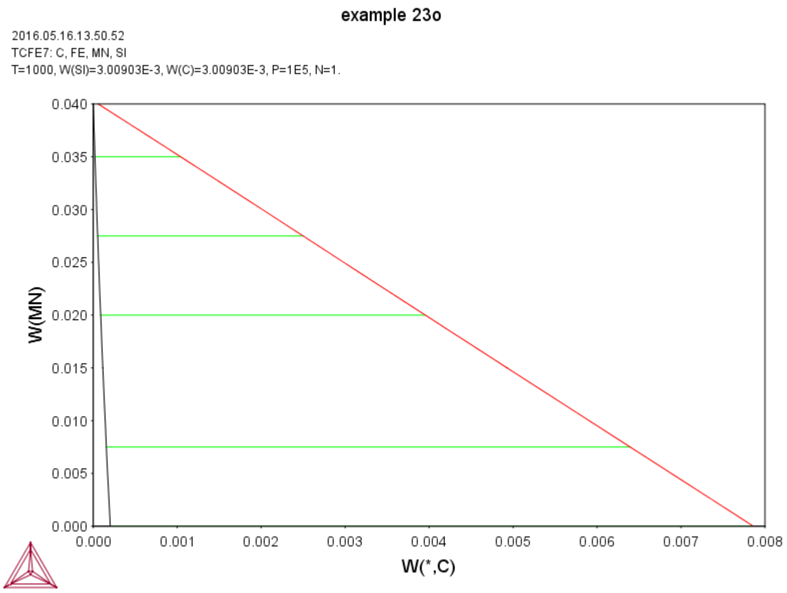


```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: @@ Calculate the corresponing para-equilibrium diagram
POLY_3: @@ where fcc and bcc have the same alloy composition.
POLY_3: read tcex23d
   ... the command in full is READ_WORKSPACES
POLY_3: @@ Only one axis is set, the interstitial composition
POLY_3: @@ must not be an axis
POLY_3: s-a-v 1 w(mn) 0 .1,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex23e y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: ?
 The following options are available:
 NORMAL             Stepping with given conditions
 INITIAL_EQUILIBRIA An initial equilibrium stored at every step
 EVALUATE           Specified variables evaluated after each step
 SEPARATE_PHASES    Each phase calculated separately
 T-ZERO             T0 line calculation
 PARAEQUILIBRIUM    Paraequilibrium diagram
 MIXED_SCHEIL       Scheil with fast diffusing elements
 ONE_PHASE_AT_TIME  One phase at a time
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
```

```
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from   0.150000E-01 for:
     BCC_A2
     FCC_A1
   1.500000E-02    0.598    0.402   2.295618E-02   5.304752E-04  -1.881771E+00
   1.250000E-02    0.542    0.458   2.524490E-02   5.935358E-04  -1.753638E+00
   1.000000E-02    0.494    0.506   2.753767E-02   6.587191E-04  -1.633619E+00
   7.500000E-03    0.454    0.546   2.983359E-02   7.260508E-04  -1.520467E+00
   5.000000E-03    0.420    0.580   3.213187E-02   7.955567E-04  -1.413204E+00
   2.500000E-03    0.390    0.610   3.443178E-02   8.672626E-04  -1.311054E+00
   2.500000E-09    0.363    0.637   3.673267E-02   9.411946E-04  -1.213385E+00

 Phase Region from   0.150000E-01 for:
     BCC_A2
     FCC_A1
   1.500000E-02    0.598    0.402   2.295989E-02   5.306073E-04  -1.881370E+00
   1.750000E-02    0.667    0.333   2.067628E-02   4.696395E-04  -2.019223E+00
   2.000000E-02    0.752    0.248   1.839858E-02   4.107379E-04  -2.169018E+00
   2.250000E-02    0.862    0.138   1.612841E-02   3.538881E-04  -2.333767E+00
   2.500000E-02    1.006   -0.006   1.386691E-02   2.990604E-04  -2.517864E+00
   2.750000E-02    1.205   -0.205   1.161307E-02   2.461731E-04  -2.728233E+00
   3.000000E-02    1.501   -0.501   9.357235E-03   1.949519E-04  -2.977273E+00
   3.250000E-02    1.985   -0.985   7.097179E-03   1.453158E-04  -3.286868E+00
   3.500000E-02    2.925   -1.925   4.831565E-03   9.721155E-05  -3.704636E+00
   3.750000E-02    5.540   -4.540   2.558996E-03   5.058863E-05  -4.373542E+00
   4.000000E-02   51.139  -50.139   2.780008E-04   5.399171E-06  -6.626764E+00
 *** Buffer savend on file
 c:\jenkins\WORKSP~1\THERMO~1\examples\tcex23\TC9F56~1.POL

 *** ERROR      8 IN NS01AD
 *** Numerical error
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: s-t-s 3
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 23n
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



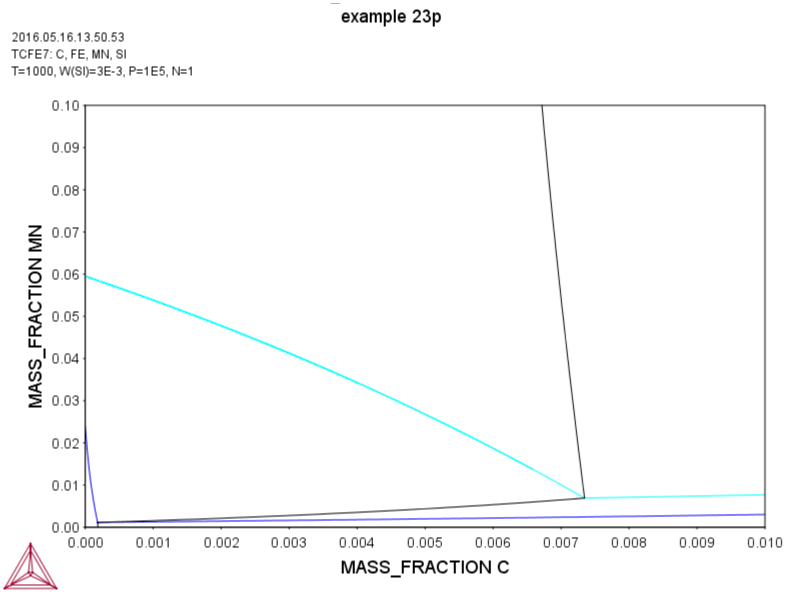
```
POST:
POST:Hit RETURN to continue
POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: set-title example 23o
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



example 23o

2016.05.16.13.50.52
TCFE7: C, FE, MN, SI
T=1000, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.

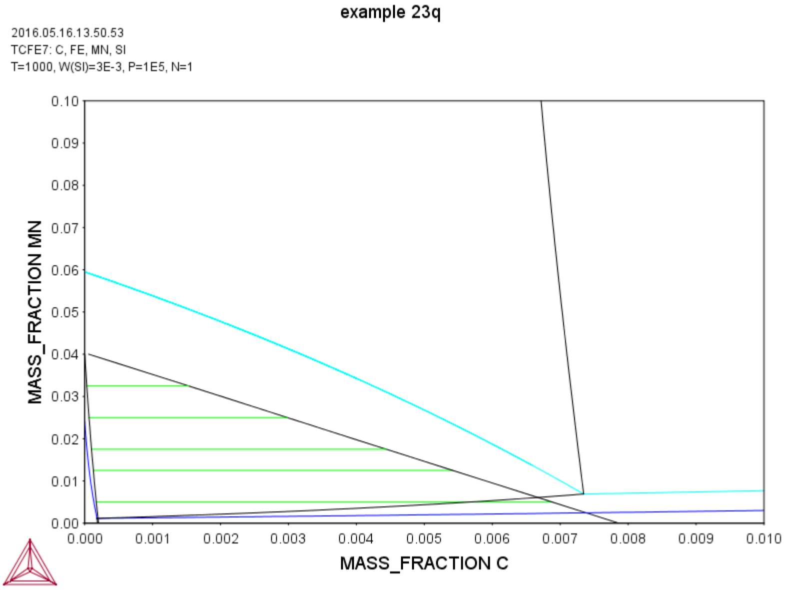
```
POST:
POST: make tcex23e y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: @@ Now overlay the two diagrams
POLY_3: read tcex23d
   ... the command in full is READ_WORKSPACES
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: set-title example 23p
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



example 23p

2016.05.16.13.50.53
TCFE7: C, FE, MN, SI
T=1000, W(SI)=3E-3, P=1E5, N=1

```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23e
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23q
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex24

About

```
 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016
```

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex24\tcex24.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Simulation of the silicon arc furnace using the REACTOR module
SYS: @@
SYS: @@ This is a very simple reactor model with output of gases at the top
SYS: @@ and output of condensed phases at the bottom. The gas phase from
SYS: @@ one segment will flow to higher segments, 80 % will react in the
SYS: @@ first above, 15% in the second above and 5 % in the third above.
SYS: @@ The condensed phases will flow downwards and all of it will go
SYS: @@ to the next lowest segment.
SYS: @@ Heat can be added at any module. The only way to specify the
SYS: @@ initial state of the reactants added to the reactor is to specify
SYS: @@ their heat content.
SYS: @@
SYS: @@ First fetch data
SYS: GO DAT
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: SW SSUB5
 Current database: SGTE Substances Database v5.1

 VA  DEFINED
TDB_SSUB5:
TDB_SSUB5: @@ Define-species means that data for just these species will be retrieved
TDB_SSUB5: @@ Define-system would mean that data for all combinations of the elements
TDB_SSUB5: @@ would be retrieved and this is not necessary here.
TDB_SSUB5: DEF-SPECIES C C1O1 C1O2 C1SI1 C2 C3 N1O1 N2 N4SI3
 C                       C1O1                    C1O2
 C1SI1                   C2                      C3
 N1O1                    N2                      N4SI3
   DEFINED
TDB_SSUB5: DEF-SP O O2 SI O1SI1 O2SI1
 O                       O2                      SI
 O1SI1                   O2SI1  DEFINED
TDB_SSUB5: GET
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
      C1<G> C<G>
   C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      C1O1<G> CO<G>
      CARBON MONOXIDE <GAS>
      STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
   C1O2<G> T.C.R.A.S. Class: 2
      C1O2<G> CO2<G>
      CARBON DIOXIDE <GAS>
   C1SI1<G> T.C.R.A.S. Class: 5
      C1SI1<G> SiC<G>
      SILICON CARBIDE <GAS>
   C2<G> T.C.R.A.S. Class: 2
      C2<G>
      CARBON Diatomic Gas.
   C3<G> T.C.R.A.S. Class: 6
      C3<G>
      CARBON <TRIATOMIC GAS>
   N1O1<G> T.C.R.A.S. Class: 1
      N1O1<G> NO<G>
      NITRIC OXIDE <GAS>
   N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      N2<G> N2<G>
      NITROGEN <DIATOMIC GAS>
      PUBLISHED BY JANAF AT 09/65
   O1<G> TCRAS 02/06/80
      O1<G> O<G>
   O1SI1<G> T.C.R.A.S. Class: 1
      O1SI1<G> SiO<G>
      SILICON <MONOXIDE GAS>
   O2<G> TCRAS 21/06/90
      O2<G>
      OXYGEN Gaseous Standard State.
   O2SI1<G> T.C.R.A.S. Class: 5
      O2SI1<G> SiO2<G>
      SILICON DIOXIDE <GAS>
   SI1<G> T.C.R.A.S. Class: 1
      SI1<G> Si<G>
      SILICON <GAS>
   O2SI1<BETA-QUARTZ> N.P.L.
      O2SI1_BETA_QUARTZ SiO2_BETA_QUARTZ
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      system by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   C1SI1<C1SI1_ALPHA> JANAF THERMOCHEMICAL TABLES SGTE **
      C1SI1_ALPHA SiC_ALPHA
      N CARBIDE <ALPHA>
      ALPHA-SIC . HEX.FORM . PUBL. BY JANAF AT 3/67 .LESS STABLE THAN
      SIC_BETA UP TO 2200K. Decomposes to complex vapour at about 3259K.
   C1SI1<C1SI1_BETA> JANAF THERMOCHEMICAL TABLES SGTE
      C1SI1_BETA SiC_BETA
      N CARBIDE <BETA>
      CUBIC FORM OF TYPE ZNS. STABLE WITH RESPECT TO SIC-ALPHA UP TO 2200K.
      PUBL. BY JANAF 03/67
   O2SI1<CRISTOBALITE> N.P.L.
      O2SI1_CRISTOBALITE SiO2_CRISTOBALITE
```

```
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   C1<DIAMOND> S.G.T.E. **
      C_DIAMOND
      <DIAMOND>
      Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
      from 1994 database (ex THERMODATA 01/93)
   C1<GRAPHITE> S.G.T.E. **
      C_GRAPHITE
      Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
   N4SI3 CHATILLON(1997)
      N4SI3 Si3N4
      Gurvich V.V., Veyts I.V., Alcock C.B., Thermodynamical Properties of
      Individual Substances,4th ed. Vol 1 and 2 English Ed (1990). S(298)
      corrected according to Koshchenko V.I., Grindberg Ya. Zh. Inorg.
      Mater.
      18(6) 903-5 (1982). Recent calorimetric determination par O'Hare et
      al., J. Mater. Res., 12 (1997) 3203-3205. Enthalpy of transformation
      alpha to beta very small(1 +- 4 kJ/ mol ) but no knowledge of T trans.
      according to them.
   O2SI1<QUARTZ> N.P.L.
      O2SI1_QUARTZ SiO2_Quartz SiO2_Alpha_Quartz
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   O2SI1<SIO2_LIQUID> N.P.L.
      O2SI1_LIQUID SiO2_Liquid
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   SI1 JANAF THERMOCHEMICAL TABLES SGTE **
      SI1 Si
      SILICON
      PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
      --U.D. 31/10/85
   O2SI1<TRIDYMITE> N.P.L.
      O2SI1_TRIDYMITE SiO2_TRIDYMITE
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
 -OK-
TDB_SSUB5: GO G
 GIBBS ENERGY SYSTEM version  5.2
GES: CH-ST EL Y VA
 ELEMENT VA                        SUSPENDED
 SPECIES VA                        SUSPENDED
GES: L-ST
 GAS CONSTANT IN USER ENERGY UNITS:      8.31451000E+00
 1 BAR IN USER PRESSURE UNITS:           1.00000000E+05
 CURRENT VALUE OF TEMPERATURE (KELVIN):          298.15
 CURRENT VALUE OF PRESSURE (PASCAL):     1.00000000E+05

 CURRENT NUMBER OF ELEMENT     4

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00 E0000000
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00 E0000000
  1 C    GRAPHITE                  1.2011E+01  1.0540E+03  5.7400E+00 08000000
  2 N    1/2_MOLE_N2(GAS)          1.4007E+01  4.3350E+03  9.5751E+01 08000000
  3 O    1/2_MOLE_O2(GAS)          1.5999E+01  4.3410E+03  1.0252E+02 08000000
  4 SI   DIAMOND_A4                2.8085E+01  3.2175E+03  1.8820E+01 08000000

 CURRENT NUMBER OF PHASE      17

 PHASE                           STATUS   SUBLATTICES
   1 GAS                         88200000     1
   2 BETA_QUARTZ                 82200000     1
   3 C1SI1_ALPHA                 82200000     1
   4 C1SI1_BETA                  82200000     1
   5 CRISTOBALITE                82200000     1
   6 DIAMOND                     82200000     1
   7 GRAPHITE                    82200000     1
   8 GRAPHITE_L                  82200000     1
   9 N4SI3_S                     82200000     1
  10 QUARTZ                      82200000     1
  11 QUARTZ_S2                   82200000     1
  12 SIO2_LIQUID                 82200000     1
  13 SI_L                        82200000     1
  14 SI_S                        82200000     1
  15 TRIDYMITE                   82200000     1
  16 TRIDYMITE_S2                82200000     1
  17 TRIDYMITE_S3                82200000     1

 CURRENT NUMBER OF SPECIES    15

 SPECIES                                    STOICHIOMETRY
   1 C                            80800000   C
   2 C1O1                         00000000   C1O1
   3 C1O2                         00000000   C1O2
   4 C1SI1                        00000000   C1SI1
   5 C2                           00000000   C2
   6 C3                           00000000   C3
   7 N                            80800000   N
   8 N1O1                         00000000   N1O1
   9 N2                           00000000   N2
  10 N4SI3                        00000000   N4SI3
  11 O                            80800000   O
  12 O1SI1                        00000000   O1SI1
  13 O2                           00000000   O2
  14 O2SI1                        00000000   O2SI1
  15 SI                           80800000   SI
  16 VA                           D1800000   VA

GES: GO R

 Thermo-Calc REACTOR version 1.0
REACTOR: ?
 AMEND_INPUT               CREATE_STAGE_BOXES        LIST_RECORDS
 AMEND_RECORD              EQUILIBRATE               MACRO-FILE-OPEN
 BACK                      EXECUTE_POLY3_COMMAND     READ_WORKSPACE
 CHANGE_SURROUNDINGS       EXIT                      SAVE_WORKSPACE
 CONTINUE_SIMULATION       GOTO_MODULE               SET_INTERACTIVE
 CREATE_DIVIDERS           HELP                      SHOW_PROBE
 CREATE_PIPES              INFORMATION               START_SIMULATION
 CREATE_PROBE              LIST_DESIGN
```

```
REACTOR: @@ Create a reactor with 4 segments which is heat controlled.
REACTOR: @@ At the top segment 1 mole of quartz (SiO2) and 1.8 mole of graphite (C)
REACTOR: @@ is added. A small amount of N is also added to simplify calculations.
REACTOR: @@ The reactants have room temperature.
REACTOR: @@ In the other three segments only heat is added.
REACTOR: @@
REACTOR: @@ A guess of the initial temperature in each segment must be provided.
REACTOR: @@
REACTOR: CREATE_STAGE
NUMBER OF STAGE BOXES /4/: 4
 YOU MUST FIRST DEFINE FEED FROM SURROUNDINGS!
GIVE FEED TO SYSTEM: N(C)=1.8
Input temperature /298.15/:
GIVE FEED TO SYSTEM: N(O2SI1)=1
Input temperature /298.15/:
GIVE FEED TO SYSTEM: H=876000
GIVE FEED TO SYSTEM: N(N2)=4e-4
Input temperature /298.15/:
GIVE FEED TO SYSTEM:

 GIVE FOR STAGE BOX     1
NAME: /SEGMENT_1/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 1750
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

 GIVE FOR STAGE BOX     2
NAME: /SEGMENT_2/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 1900
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

 GIVE FOR STAGE BOX     3
NAME: /SEGMENT_3/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 2050
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

 GIVE FOR STAGE BOX     4
NAME: /SEGMENT_4/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 2200
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST
REACTOR: l-r

 Number:  0 name: SURROUNDINGS             stage box at:    23,
 Feed of C                        with  1.8000E+00 mol to record:    -1
 Feed of O2SI1                    with  1.0000E+00 mol to record:    -1
 Feed of heat  8.7600E+05 J to record:    -1
 Feed of N2                       with  4.0000E-04 mol to record:    -1

 Number:  1 name: SEGMENT_1                stage box at:    72, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:  2 name: SEGMENT_2                stage box at:   114, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:  3 name: SEGMENT_3                stage box at:   156, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:  4 name: SEGMENT_4                stage box at:   198, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1
REACTOR: @@ Create dividers, one for distributing the gas from segment 2 to 4
REACTOR: @@ one for splitting the heat feed and one for splitting the feed on N2
REACTOR: create-div
Number of dividers /4/: 5
Number of outputs for divider 1: /3/: 2
Percent of input to output 1: /100/: 80
Number of outputs for divider 2: /3/: 3
Percent of input to output 1: /100/: 80 15
Number of outputs for divider 3: /3/: 3
Percent of input to output 1: /100/: 80 15
Number of outputs for divider 4: /3/: 3
Percent of input to output 1: /100/: 85 10
Number of outputs for divider 5: /3/: 4
Percent of input to output 1: /100/: 25 25 25
REACTOR: l-r

 Number:  0 name: SURROUNDINGS             stage box at:    23,
 Feed of C                        with  1.8000E+00 mol to record:    -1
 Feed of O2SI1                    with  1.0000E+00 mol to record:    -1
 Feed of heat  8.7600E+05 J to record:    -1
 Feed of N2                       with  4.0000E-04 mol to record:    -1

 Number:  1 name: SEGMENT_1                stage box at:    72, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:  2 name: SEGMENT_2                stage box at:   114, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1
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 Number:  3 name: SEGMENT_3                stage box at:   156, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:  4 name: SEGMENT_4                stage box at:   198, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:   5 name: DIVIDER_5                divider at:   240
   80 % of input to record:   -1
   20 % of input to record:   -1

 Number:   6 name: DIVIDER_6                divider at:   268
   80 % of input to record:   -1
   15 % of input to record:   -1
    5 % of input to record:   -1

 Number:   7 name: DIVIDER_7                divider at:   301
   80 % of input to record:   -1
   15 % of input to record:   -1
    5 % of input to record:   -1

 Number:   8 name: DIVIDER_8                divider at:   334
   85 % of input to record:   -1
   10 % of input to record:   -1
    5 % of input to record:   -1

 Number:   9 name: DIVIDER_9                divider at:   367
   25 % of input to record:   -1
   25 % of input to record:   -1
   25 % of input to record:   -1
   25 % of input to record:   -1
REACTOR: @@ Finally create the pipes between the segments first for the feed
REACTOR: c-pipe 0 1 1 8 9
 Feed of C
 Feed of O2SI1
 Feed of heat
 Input set to this divider
 Feed of N2
 Input set to this divider
 NO MORE OUTPUT RECORDS
REACTOR: @@ All solid phases are assumed to go down one segment
REACTOR: @@ The gas phase is assumed to go up, 80% to the next segment,
REACTOR: @@ 15% to the second next and 5% to the third segment above.
REACTOR: @@ output from stage boxes
REACTOR: c-pipe 1 0 2
 Output record for phase GAS
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 2 5 3
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 3 6 4
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 4 7 0
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: @@ output from dividers
REACTOR: c-pipe 5 1 0
 Output record for   80 % of input
 Output record for   20 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 6 2 1 0
 Output record for   80 % of input
 Output record for   15 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 7 3 2 1
 Output record for   80 % of input
 Output record for   15 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 8 4 3 2
 Output record for   85 % of input
 Output record for   10 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 9 1 2 3 4
 Output record for   25 % of input
 Output record for   25 % of input
 Output record for   25 % of input
 Output record for   25 % of input
 NO MORE OUTPUT RECORDS
REACTOR: l-r

 Number:  0 name: SURROUNDINGS             stage box at:    23,
 Feed of C                        with  1.8000E+00 mol to record:     1
 Feed of O2SI1                    with  1.0000E+00 mol to record:     1
 Feed of heat  8.7600E+05 J to record:     8
 Feed of N2                       with  4.0000E-04 mol to record:     9

 Number:  1 name: SEGMENT_1                stage box at:    72, H controlled
 Output for phase GAS                      to record:    0
 Output for phase REST                     to record:    2

 Number:  2 name: SEGMENT_2                stage box at:   114, H controlled
 Output for phase GAS                      to record:    5
 Output for phase REST                     to record:    3

 Number:  3 name: SEGMENT_3                stage box at:   156, H controlled
 Output for phase GAS                      to record:    6
 Output for phase REST                     to record:    4

 Number:  4 name: SEGMENT_4                stage box at:   198, H controlled
 Output for phase GAS                      to record:    7
 Output for phase REST                     to record:    0

 Number:   5 name: DIVIDER_5                divider at:   240
```

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   80 % of input to record:    1
   20 % of input to record:    0

 Number:    6 name: DIVIDER_6                divider at:   268
   80 % of input to record:    2
   15 % of input to record:    1
    5 % of input to record:    0

 Number:    7 name: DIVIDER_7                divider at:   301
   80 % of input to record:    3
   15 % of input to record:    2
    5 % of input to record:    1

 Number:    8 name: DIVIDER_8                divider at:   334
   85 % of input to record:    4
   10 % of input to record:    3
    5 % of input to record:    2

 Number:    9 name: DIVIDER_9                divider at:   367
   25 % of input to record:    1
   25 % of input to record:    2
   25 % of input to record:    3
   25 % of input to record:    4
REACTOR: save tcex24 y
REACTOR: @@ Now start the process
REACTOR: read tcex24
REACTOR:
REACTOR: @@ The output for each iteration will consist of the conditions set in
REACTOR: @@ each segment, and the user may select some state variables also,
REACTOR: @@ in this case NP($) meaning moles of stable phases
REACTOR: @@ After each loop the temperatures in all segments are listed
REACTOR: @@
REACTOR: @@ We want to achive a reactor where only Si<L> leaves at the bottom.
REACTOR: START
Max number of loops: /10/: 50
OUTPUT TO SCREEN OR FILE /SCREEN/:
Output conditions? /Y/:
Output variables: /T BP($)/: T BP($)
 >>> DATA AT ITERATION    1 FROM STAGE    1
 T=1750, P=1E5, N(C)=1.8, N(N)=2E-4, N(O)=2, N(SI)=1
 DEGREES OF FREEDOM 0
T= 1.750000E+03
 BP(GAS)=8.3899239E-3, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=3.9560636E-3, BP(CRISTOBALITE)=60.077021, BP(DIAMOND)=0,
    BP(GRAPHITE)=21.616235, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    1 FROM STAGE    2
 T=1900, P=1E5, N(C)=1.7998, N(N)=2E-4, N(O)=1.9998, N(SI)=0.999999
 DEGREES OF FREEDOM 0
T= 1.900000E+03
 BP(GAS)=35.781375, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.515817, BP(CRISTOBALITE)=22.402821, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    1 FROM STAGE    3
 T=2050, P=1E5, N(C)=0.586488, N(N)=2E-4, N(O)=0.745729, N(SI)=0.959352
 DEGREES OF FREEDOM 0
T= 2.050000E+03
 BP(GAS)=1.1001909E-2, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.51327, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=22.396537, BP(SI_L)=6.3106228E-4,
    BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    1 FROM STAGE    4
 T=2200, P=1E5, N(C)=0.586424, N(N)=2E-4, N(O)=0.74552, N(SI)=0.959207
 DEGREES OF FREEDOM 0
T= 2.200000E+03
 BP(GAS)=27.369406, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=9.7781171, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=8.7657159, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    2 FROM STAGE    1
 H=-9.69232E5, P=1E5, N(C)=2.78779, N(N)=4E-4, N(O)=3.04056, N(SI)=1.0527
 DEGREES OF FREEDOM 0
T= 1.098651E+03
 BP(GAS)=25.395955, BP(BETA_QUARTZ)=63.249404, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=0, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=23.055463, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    2 FROM STAGE    2
 H=-8.37416E5, P=1E5, N(C)=1.97096, N(N)=3.9E-4, N(O)=2.2174, N(SI)=1.1133
 DEGREES OF FREEDOM 0
T= 1.764644E+03
 BP(GAS)=2.577188E-2, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=0.19891753, BP(CRISTOBALITE)=66.592185, BP(DIAMOND)=0,
    BP(GRAPHITE)=23.605007, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    2 FROM STAGE    3
 H=-7.72457E5, P=1E5, N(C)=2.24429, N(N)=3.6E-4, N(O)=2.81309, N(SI)=1.43588
 DEGREES OF FREEDOM 0
T= 1.785830E+03
 BP(GAS)=28.121362, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=21.054185, BP(CRISTOBALITE)=54.435284, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.6836041, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    2 FROM STAGE    4
 H=33660.3, P=1E5, N(C)=1.24807, N(N)=2E-4, N(O)=1.812, N(SI)=1.4311
 DEGREES OF FREEDOM 0
T= 2.447572E+03
 BP(GAS)=60.210327, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=0.5584779, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=23.40707, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    3 FROM STAGE    1
 H=-9.22751E5, P=1E5, N(C)=2.01172, N(N)=5.76E-4, N(O)=2.24134, N(SI)=1.02991
 DEGREES OF FREEDOM 0
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T= 8.124883E+02
 BP(GAS)=4.0693569, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=23.005715,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=61.879868, BP(QUARTZ_S2)=0,
    BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    3 FROM STAGE    2
 H=-9.0397E5, P=1E5, N(C)=2.89749, N(N)=5.18E-4, N(O)=3.13248, N(SI)=1.12129
 DEGREES OF FREEDOM 0
T= 1.746338E+03
 BP(GAS)=25.042951, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=67.278274, BP(DIAMOND)=0, BP(GRAPHITE)=24.095798,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
    BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    3 FROM STAGE    3
 H=-8.04917E5, P=1E5, N(C)=2.99345, N(N)=3.6E-4, N(O)=3.68911, N(SI)=1.58674
 DEGREES OF FREEDOM 0
T= 1.785838E+03
 BP(GAS)=55.589669, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=28.960504, BP(CRISTOBALITE)=51.37138, BP(DIAMOND)=0,
    BP(GRAPHITE)=3.6235819, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    3 FROM STAGE    4
 H=61307.1, P=1E5, N(C)=1.02397, N(N)=2E-4, N(O)=1.71001, N(SI)=1.57729
 DEGREES OF FREEDOM 0
T= 2.594647E+03
 BP(GAS)=59.391022, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=24.567245, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    4 FROM STAGE    1
 H=-9.75673E5, P=1E5, N(C)=2.8597, N(N)=6.784E-4, N(O)=3.09674, N(SI)=1.03777
 DEGREES OF FREEDOM 0
T= 1.067994E+03
 BP(GAS)=27.303365, BP(BETA_QUARTZ)=62.352571, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=0, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=23.392027, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    4 FROM STAGE    2
 H=-9.26156E5, P=1E5, N(C)=3.67673, N(N)=5.18E-4, N(O)=3.91533, N(SI)=1.15072
 DEGREES OF FREEDOM 0
T= 1.785833E+03
 BP(GAS)=48.987037, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=2.2730168, BP(CRISTOBALITE)=65.232008, BP(DIAMOND)=0,
    BP(GRAPHITE)=22.635726, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    4 FROM STAGE    3
 H=-7.59974E5, P=1E5, N(C)=2.76045, N(N)=3.6E-4, N(O)=3.53941, N(SI)=1.70442
 DEGREES OF FREEDOM 0
T= 1.856422E+03
 BP(GAS)=54.420155, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.739066, BP(CRISTOBALITE)=48.49715, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    4 FROM STAGE    4
 H=97718.1, P=1E5, N(C)=0.866397, N(N)=2E-4, N(O)=1.61434, N(SI)=1.67357
 DEGREES OF FREEDOM 0
T= 2.773504E+03
 BP(GAS)=58.669424, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=24.569593, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    5 FROM STAGE    1
 H=-1.01358E6, P=1E5, N(C)=3.5158, N(N)=6.784E-4, N(O)=3.76462, N(SI)=1.05123
 DEGREES OF FREEDOM 0
T= 1.163508E+03
 BP(GAS)=45.980219, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=22.850503,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
    BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=63.161004
 >>> DATA AT ITERATION    5 FROM STAGE    2
 H=-9.1327E5, P=1E5, N(C)=3.54766, N(N)=5.18E-4, N(O)=3.88466, N(SI)=1.19572
 DEGREES OF FREEDOM 0
T= 1.785833E+03
 BP(GAS)=49.603255, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=5.1279351, BP(CRISTOBALITE)=63.651652, BP(DIAMOND)=0,
    BP(GRAPHITE)=19.968003, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    5 FROM STAGE    3
 H=-7.20023E5, P=1E5, N(C)=2.48349, N(N)=3.6E-4, N(O)=3.41026, N(SI)=1.82628
 DEGREES OF FREEDOM 0
T= 1.974923E+03
 BP(GAS)=54.111761, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=33.932787, BP(CRISTOBALITE)=47.641383, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    5 FROM STAGE    4
 H=1.21546E5, P=1E5, N(C)=0.846289, N(N)=2E-4, N(O)=1.58585, N(SI)=1.63921
 DEGREES OF FREEDOM 0
T= 2.880121E+03
 BP(GAS)=58.994116, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.582856, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    6 FROM STAGE    1
 H=-1.01075E6, P=1E5, N(C)=3.49373, N(N)=6.784E-4, N(O)=3.76565,
    N(SI)=1.07656
 DEGREES OF FREEDOM 0
T= 1.245814E+03
 BP(GAS)=44.984991, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=22.786504,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
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    BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=64.683179
 >>> DATA AT ITERATION    6 FROM STAGE    2
 H=-9.07819E5, P=1E5, N(C)=3.33384, N(N)=5.18E-4, N(O)=3.85053, N(SI)=1.35148
 DEGREES OF FREEDOM 0
T= 1.785834E+03
 BP(GAS)=49.986926, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=12.328797, BP(CRISTOBALITE)=62.215897, BP(DIAMOND)=0,
    BP(GRAPHITE)=15.079392, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    6 FROM STAGE    3
 H=-6.89982E5, P=1E5, N(C)=2.23998, N(N)=3.6E-4, N(O)=3.33968, N(SI)=2.01108
 DEGREES OF FREEDOM 0
T= 2.024859E+03
 BP(GAS)=55.901309, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=33.947223, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=46.973648, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    6 FROM STAGE    4
 H=1.42732E5, P=1E5, N(C)=0.846649, N(N)=2E-4, N(O)=1.56363, N(SI)=1.62846
 DEGREES OF FREEDOM 0
T= 2.939413E+03
 BP(GAS)=59.078725, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=21.844947, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 =================================
 >>> DATA AT ITERATION    7 FROM STAGE    1
 H=-1.00894E6, P=1E5, N(C)=3.46804, N(N)=6.784E-4, N(O)=3.76822,
    N(SI)=1.10673
 DEGREES OF FREEDOM 0
T= 1.360090E+03
 BP(GAS)=43.509998, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=23.028873,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
    BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=66.495404
 >>> DATA AT ITERATION    7 FROM STAGE    2
 H=-9.0846E5, P=1E5, N(C)=3.15898, N(N)=5.18E-4, N(O)=3.86884, N(SI)=1.54042
 DEGREES OF FREEDOM 0
T= 1.785834E+03
 BP(GAS)=51.714964, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=20.759112, BP(CRISTOBALITE)=60.917489, BP(DIAMOND)=0,
    BP(GRAPHITE)=9.7183695, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    7 FROM STAGE    3
 H=-6.68401E5, P=1E5, N(C)=2.00418, N(N)=3.6E-4, N(O)=3.27868, N(SI)=2.21214
 DEGREES OF FREEDOM 0
T= 2.054719E+03
 BP(GAS)=58.391066, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.178134, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=46.091552, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    7 FROM STAGE    4
 H=1.5752E5, P=1E5, N(C)=0.852408, N(N)=2E-4, N(O)=1.53426, N(SI)=1.61954
 DEGREES OF FREEDOM 0
T= 2.970399E+03
 BP(GAS)=58.350803, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=21.921684, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 =================================
 >>> DATA AT ITERATION    8 FROM STAGE    1
 H=-1.01026E6, P=1E5, N(C)=3.48108, N(N)=6.784E-4, N(O)=3.81122,
    N(SI)=1.13788
 DEGREES OF FREEDOM 0
T= 1.482989E+03
 BP(GAS)=43.00392, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=23.382925,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
    BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=68.366928
 >>> DATA AT ITERATION    8 FROM STAGE    2
 H=-9.10878E5, P=1E5, N(C)=2.99607, N(N)=5.18E-4, N(O)=3.90142, N(SI)=1.7378
 DEGREES OF FREEDOM 0
T= 1.785834E+03
 BP(GAS)=53.79187, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=29.488666, BP(CRISTOBALITE)=59.674773, BP(DIAMOND)=0,
    BP(GRAPHITE)=4.262819, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    8 FROM STAGE    3
 H=-6.55233E5, P=1E5, N(C)=1.77229, N(N)=3.6E-4, N(O)=3.21382, N(SI)=2.39985
 DEGREES OF FREEDOM 0
T= 2.072919E+03
 BP(GAS)=59.871555, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.480045, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=45.758102, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    8 FROM STAGE    4
 H=1.63921E5, P=1E5, N(C)=0.859937, N(N)=2E-4, N(O)=1.52316, N(SI)=1.62152
 DEGREES OF FREEDOM 0
T= 2.980408E+03
 BP(GAS)=57.971017, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.269931, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 =================================
 >>> DATA AT ITERATION    9 FROM STAGE    1
 H=-1.01265E6, P=1E5, N(C)=3.50442, N(N)=6.784E-4, N(O)=3.86176, N(SI)=1.1655
 DEGREES OF FREEDOM 0
T= 1.587698E+03
 BP(GAS)=42.882393, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=23.711015,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
    BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=70.024973
 >>> DATA AT ITERATION    9 FROM STAGE    2
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 H=-9.13276E5, P=1E5, N(C)=2.83298, N(N)=5.18E-4, N(O)=3.91194, N(SI)=1.91242
 DEGREES OF FREEDOM 0
T= 1.813659E+03
 BP(GAS)=54.528551, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=36.500134, BP(CRISTOBALITE)=59.303002, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    9 FROM STAGE    3
 H=-6.54501E5, P=1E5, N(C)=1.59827, N(N)=3.6E-4, N(O)=3.19257, N(SI)=2.56019
 DEGREES OF FREEDOM 0
T= 2.082775E+03
 BP(GAS)=61.270691, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.761699, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=46.15036, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    9 FROM STAGE    4
 H=1.60038E5, P=1E5, N(C)=0.866962, N(N)=2E-4, N(O)=1.53622, N(SI)=1.63507
 DEGREES OF FREEDOM 0
T= 2.968716E+03
 BP(GAS)=58.165846, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.749015, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   10 FROM STAGE    1
 H=-1.01175E6, P=1E5, N(C)=3.49117, N(N)=6.784E-4, N(O)=3.87559,
    N(SI)=1.19209
 DEGREES OF FREEDOM 0
T= 1.688378E+03
 BP(GAS)=41.818997, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=24.015589,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
    BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=71.592751
 >>> DATA AT ITERATION   10 FROM STAGE    2
 H=-9.17571E5, P=1E5, N(C)=2.71456, N(N)=5.18E-4, N(O)=3.93864, N(SI)=2.05542
 DEGREES OF FREEDOM 0
T= 1.931654E+03
 BP(GAS)=54.443868, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.245343, BP(CRISTOBALITE)=61.663362, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   10 FROM STAGE    3
 H=-6.75806E5, P=1E5, N(C)=1.62247, N(N)=3.6E-4, N(O)=3.28158, N(SI)=2.61526
 DEGREES OF FREEDOM 0
T= 2.082796E+03
 BP(GAS)=62.678063, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.079061, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=47.68706, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   10 FROM STAGE    4
 H=1.40325E5, P=1E5, N(C)=0.874877, N(N)=2E-4, N(O)=1.58737, N(SI)=1.66856
 DEGREES OF FREEDOM 0
T= 2.917962E+03
 BP(GAS)=59.278419, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=23.490504, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   11 FROM STAGE    1
 H=-1.00311E6, P=1E5, N(C)=3.3844, N(N)=6.784E-4, N(O)=3.84233, N(SI)=1.26378
 DEGREES OF FREEDOM 0
T= 1.785825E+03
 BP(GAS)=40.181412, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=2.0429794, BP(CRISTOBALITE)=72.460051, BP(DIAMOND)=0,
    BP(GRAPHITE)=22.941883, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   11 FROM STAGE    2
 H=-9.22617E5, P=1E5, N(C)=2.69033, N(N)=5.18E-4, N(O)=4.00547, N(SI)=2.13913
 DEGREES OF FREEDOM 0
T= 1.964263E+03
 BP(GAS)=56.690324, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.355782, BP(CRISTOBALITE)=62.435822, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   11 FROM STAGE    3
 H=-6.99253E5, P=1E5, N(C)=1.63156, N(N)=3.6E-4, N(O)=3.34822, N(SI)=2.63654
 DEGREES OF FREEDOM 0
T= 2.082357E+03
 BP(GAS)=62.812321, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.943937, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=49.460883, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   11 FROM STAGE    4
 H=1.17365E5, P=1E5, N(C)=0.871507, N(N)=2E-4, N(O)=1.64642, N(SI)=1.69472
 DEGREES OF FREEDOM 0
T= 2.855981E+03
 BP(GAS)=60.986549, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=23.421073, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   12 FROM STAGE    1
 H=-1.00345E6, P=1E5, N(C)=3.36452, N(N)=6.784E-4, N(O)=3.87931,
    N(SI)=1.31896
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=41.745842, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=4.6200248, BP(CRISTOBALITE)=71.897832, BP(DIAMOND)=0,
    BP(GRAPHITE)=21.265337, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   12 FROM STAGE    2
 H=-9.23112E5, P=1E5, N(C)=2.62448, N(N)=5.18E-4, N(O)=4.00169, N(SI)=2.19444
 DEGREES OF FREEDOM 0
T= 1.981583E+03
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 BP(GAS)=56.956864, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.363041, BP(CRISTOBALITE)=62.863929, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   12 FROM STAGE    3
 H=-7.19679E5, P=1E5, N(C)=1.62905, N(N)=3.6E-4, N(O)=3.4097, N(SI)=2.66675
 DEGREES OF FREEDOM 0
T= 2.082497E+03
 BP(GAS)=63.219192, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.784904, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=51.014914, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   12 FROM STAGE    4
 H=97299.2, P=1E5, N(C)=0.867541, N(N)=2E-4, N(O)=1.69815, N(SI)=1.71661
 DEGREES OF FREEDOM 0
T= 2.791245E+03
 BP(GAS)=62.594968, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=23.207652, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   13 FROM STAGE    1
 H=-1.00205E6, P=1E5, N(C)=3.31172, N(N)=6.784E-4, N(O)=3.86893,
    N(SI)=1.36009
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=41.7826, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=6.5030761, BP(CRISTOBALITE)=71.546701, BP(DIAMOND)=0,
    BP(GRAPHITE)=20.051342, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   13 FROM STAGE    2
 H=-9.24576E5, P=1E5, N(C)=2.57094, N(N)=5.18E-4, N(O)=4.00556, N(SI)=2.24663
 DEGREES OF FREEDOM 0
T= 1.994519E+03
 BP(GAS)=57.417428, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.390387, BP(CRISTOBALITE)=63.260705, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   13 FROM STAGE    3
 H=-7.374E5, P=1E5, N(C)=1.62655, N(N)=3.6E-4, N(O)=3.4643, N(SI)=2.69763
 DEGREES OF FREEDOM 0
T= 2.082731E+03
 BP(GAS)=63.654312, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.710227, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=52.365328, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   13 FROM STAGE    4
 H=79895.2, P=1E5, N(C)=0.865678, N(N)=2E-4, N(O)=1.7431, N(SI)=1.73723
 DEGREES OF FREEDOM 0
T= 2.721648E+03
 BP(GAS)=64.038962, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=23.039395, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   14 FROM STAGE    1
 H=-1.00119E6, P=1E5, N(C)=3.26815, N(N)=6.784E-4, N(O)=3.86516,
    N(SI)=1.39888
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=41.977202, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=8.2717561, BP(CRISTOBALITE)=71.225272, BP(DIAMOND)=0,
    BP(GRAPHITE)=18.915409, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   14 FROM STAGE    2
 H=-9.25814E5, P=1E5, N(C)=2.51969, N(N)=5.18E-4, N(O)=4.00932, N(SI)=2.2976
 DEGREES OF FREEDOM 0
T= 2.001975E+03
 BP(GAS)=56.899727, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.678344, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=64.366461, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   14 FROM STAGE    3
 H=-7.5344E5, P=1E5, N(C)=1.63225, N(N)=3.6E-4, N(O)=3.53706, N(SI)=2.7445
 DEGREES OF FREEDOM 0
T= 2.083146E+03
 BP(GAS)=65.078538, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.68776, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=53.512479, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   14 FROM STAGE    4
 H=65149.9, P=1E5, N(C)=0.865118, N(N)=2E-4, N(O)=1.78129, N(SI)=1.75576
 DEGREES OF FREEDOM 0
T= 2.649675E+03
 BP(GAS)=65.327667, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.875373, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   15 FROM STAGE    1
 H=-9.99863E5, P=1E5, N(C)=3.22232, N(N)=6.784E-4, N(O)=3.84582,
    N(SI)=1.42466
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=41.607103, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=9.4314288, BP(CRISTOBALITE)=71.039976, BP(DIAMOND)=0,
    BP(GRAPHITE)=18.175039, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   15 FROM STAGE    2
 H=-9.28208E5, P=1E5, N(C)=2.49189, N(N)=5.18E-4, N(O)=4.03654, N(SI)=2.34977
 DEGREES OF FREEDOM 0
T= 2.011374E+03
 BP(GAS)=58.095641, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.727938, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
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    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=64.687647, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   15 FROM STAGE    3
 H=-7.66271E5, P=1E5, N(C)=1.63303, N(N)=3.6E-4, N(O)=3.5783, N(SI)=2.77058
 DEGREES OF FREEDOM 0
T= 2.083324E+03
 BP(GAS)=65.468307, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.724895, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=54.487318, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   15 FROM STAGE    4
 H=52616., P=1E5, N(C)=0.866044, N(N)=2E-4, N(O)=1.81373, N(SI)=1.77291
 DEGREES OF FREEDOM 0
T= 2.575865E+03
 BP(GAS)=66.4689, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.746115, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   16 FROM STAGE    1
 H=-1.00007E6, P=1E5, N(C)=3.19911, N(N)=6.784E-4, N(O)=3.86199,
    N(SI)=1.46355
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=42.375412, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=11.209868, BP(CRISTOBALITE)=70.703913, BP(DIAMOND)=0,
    BP(GRAPHITE)=17.036612, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   16 FROM STAGE    2
 H=-9.28527E5, P=1E5, N(C)=2.44149, N(N)=5.18E-4, N(O)=4.03726, N(SI)=2.39893
 DEGREES OF FREEDOM 0
T= 2.020037E+03
 BP(GAS)=58.591619, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.771357, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=64.935199, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   16 FROM STAGE    3
 H=-7.76568E5, P=1E5, N(C)=1.63486, N(N)=3.6E-4, N(O)=3.6125, N(SI)=2.79319
 DEGREES OF FREEDOM 0
T= 2.083472E+03
 BP(GAS)=65.828608, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.789071, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=55.266798, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   16 FROM STAGE    4
 H=42605.4, P=1E5, N(C)=0.867644, N(N)=2E-4, N(O)=1.83968, N(SI)=1.78749
 DEGREES OF FREEDOM 0
T= 2.507707E+03
 BP(GAS)=67.422071, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.6366, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   17 FROM STAGE    1
 H=-9.99181E5, P=1E5, N(C)=3.15804, N(N)=6.784E-4, N(O)=3.8585, N(SI)=1.50085
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=42.570553, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=12.913325, BP(CRISTOBALITE)=70.390441, BP(DIAMOND)=0,
    BP(GRAPHITE)=15.949972, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   17 FROM STAGE    2
 H=-9.28656E5, P=1E5, N(C)=2.39392, N(N)=5.18E-4, N(O)=4.03732, N(SI)=2.4454
 DEGREES OF FREEDOM 0
T= 2.027376E+03
 BP(GAS)=59.074267, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.816728, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.141742, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   17 FROM STAGE    3
 H=-7.84668E5, P=1E5, N(C)=1.63727, N(N)=3.6E-4, N(O)=3.64014, N(SI)=2.81254
 DEGREES OF FREEDOM 0
T= 2.083598E+03
 BP(GAS)=66.144587, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.875517, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=55.878823, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   17 FROM STAGE    4
 H=34757.6, P=1E5, N(C)=0.8698, N(N)=2E-4, N(O)=1.86005, N(SI)=1.79983
 DEGREES OF FREEDOM 0
T= 2.447966E+03
 BP(GAS)=68.189731, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.567411, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   18 FROM STAGE    1
 H=-9.98331E5, P=1E5, N(C)=3.11923, N(N)=6.784E-4, N(O)=3.85516,
    N(SI)=1.53616
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=42.754622, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=14.526169, BP(CRISTOBALITE)=70.09308, BP(DIAMOND)=0,
    BP(GRAPHITE)=14.922319, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   18 FROM STAGE    2
 H=-9.28547E5, P=1E5, N(C)=2.34912, N(N)=5.18E-4, N(O)=4.03628, N(SI)=2.4885
 DEGREES OF FREEDOM 0
T= 2.033605E+03
 BP(GAS)=59.522046, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.858508, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.307945, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
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 >>> DATA AT ITERATION   18 FROM STAGE    3
 H=-7.9095E5, P=1E5, N(C)=1.64004, N(N)=3.6E-4, N(O)=3.66197, N(SI)=2.82819
 DEGREES OF FREEDOM 0
T= 2.083688E+03
 BP(GAS)=66.403735, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.965075, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=56.352228, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   18 FROM STAGE    4
 H=28693.4, P=1E5, N(C)=0.872034, N(N)=2E-4, N(O)=1.87581, N(SI)=1.80994
 DEGREES OF FREEDOM 0
T= 2.398232E+03
 BP(GAS)=68.793565, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.52654, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   19 FROM STAGE    1
 H=-9.97507E5, P=1E5, N(C)=3.08274, N(N)=6.784E-4, N(O)=3.8516, N(SI)=1.569
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=42.913713, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=16.0268, BP(CRISTOBALITE)=69.816122, BP(DIAMOND)=0,
    BP(GRAPHITE)=13.966842, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   19 FROM STAGE    2
 H=-9.28273E5, P=1E5, N(C)=2.30776, N(N)=5.18E-4, N(O)=4.03429, N(SI)=2.52748
 DEGREES OF FREEDOM 0
T= 2.038832E+03
 BP(GAS)=59.919125, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.894909, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.440555, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   19 FROM STAGE    3
 H=-7.95775E5, P=1E5, N(C)=1.64273, N(N)=3.6E-4, N(O)=3.67899, N(SI)=2.84056
 DEGREES OF FREEDOM 0
T= 2.083751E+03
 BP(GAS)=66.611155, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.046897, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=56.715065, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   19 FROM STAGE    4
 H=24048.8, P=1E5, N(C)=0.874075, N(N)=2E-4, N(O)=1.88789, N(SI)=1.81802
 DEGREES OF FREEDOM 0
T= 2.358285E+03
 BP(GAS)=69.261131, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.503633, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   20 FROM STAGE    1
 H=-9.96727E5, P=1E5, N(C)=3.04912, N(N)=6.784E-4, N(O)=3.84782,
    N(SI)=1.59879
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.042147, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=17.387655, BP(CRISTOBALITE)=69.565062, BP(DIAMOND)=0,
    BP(GRAPHITE)=13.100767, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   20 FROM STAGE    2
 H=-9.27909E5, P=1E5, N(C)=2.27042, N(N)=5.18E-4, N(O)=4.03169, N(SI)=2.56201
 DEGREES OF FREEDOM 0
T= 2.043175E+03
 BP(GAS)=60.26286, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.925513, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.546005, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   20 FROM STAGE    3
 H=-7.99465E5, P=1E5, N(C)=1.64513, N(N)=3.6E-4, N(O)=3.69216, N(SI)=2.85019
 DEGREES OF FREEDOM 0
T= 2.083795E+03
 BP(GAS)=66.774912, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.116372, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=56.991941, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   20 FROM STAGE    4
 H=20506.2, P=1E5, N(C)=0.875807, N(N)=2E-4, N(O)=1.89711, N(SI)=1.82436
 DEGREES OF FREEDOM 0
T= 2.326902E+03
 BP(GAS)=69.620213, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.490901, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   21 FROM STAGE    1
 H=-9.96006E5, P=1E5, N(C)=3.01883, N(N)=6.784E-4, N(O)=3.84399,
    N(SI)=1.62523
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.142842, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=18.595742, BP(CRISTOBALITE)=69.342396, BP(DIAMOND)=0,
    BP(GRAPHITE)=12.332156, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   21 FROM STAGE    2
 H=-9.27508E5, P=1E5, N(C)=2.23735, N(N)=5.18E-4, N(O)=4.02883, N(SI)=2.59209
 DEGREES OF FREEDOM 0
T= 2.046761E+03
 BP(GAS)=60.555657, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.95068, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.629721, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   21 FROM STAGE    3
 H=-8.02281E5, P=1E5, N(C)=1.64714, N(N)=3.6E-4, N(O)=3.70232, N(SI)=2.85765
 DEGREES OF FREEDOM 0
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T= 2.083827E+03
 BP(GAS)=66.903686, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.172894, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.202793, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   21 FROM STAGE    4
 H=17809.2, P=1E5, N(C)=0.877217, N(N)=2E-4, N(O)=1.90413, N(SI)=1.82928
 DEGREES OF FREEDOM 0
T= 2.302569E+03
 BP(GAS)=69.894815, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.483673, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   22 FROM STAGE    1
 H=-9.95358E5, P=1E5, N(C)=2.99203, N(N)=6.784E-4, N(O)=3.84029,
    N(SI)=1.64831
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.220494, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=19.650414, BP(CRISTOBALITE)=69.148215, BP(DIAMOND)=0,
    BP(GRAPHITE)=11.661297, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   22 FROM STAGE    2
 H=-9.27105E5, P=1E5, N(C)=2.20849, N(N)=5.18E-4, N(O)=4.02593, N(SI)=2.61797
 DEGREES OF FREEDOM 0
T= 2.049708E+03
 BP(GAS)=60.802621, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.971114, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.696163, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   22 FROM STAGE    3
 H=-8.04427E5, P=1E5, N(C)=1.64878, N(N)=3.6E-4, N(O)=3.71015, N(SI)=2.86341
 DEGREES OF FREEDOM 0
T= 2.083850E+03
 BP(GAS)=67.004966, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.217743, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.363223, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   22 FROM STAGE    4
 H=15757.7, P=1E5, N(C)=0.878336, N(N)=2E-4, N(O)=1.90947, N(SI)=1.83307
 DEGREES OF FREEDOM 0
T= 2.283845E+03
 BP(GAS)=70.104344, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.479422, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   23 FROM STAGE    1
 H=-9.94784E5, P=1E5, N(C)=2.96867, N(N)=6.784E-4, N(O)=3.83684,
    N(SI)=1.66821
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.280013, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=20.559619, BP(CRISTOBALITE)=68.980974, BP(DIAMOND)=0,
    BP(GRAPHITE)=11.083055, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   23 FROM STAGE    2
 H=-9.26721E5, P=1E5, N(C)=2.18361, N(N)=5.18E-4, N(O)=4.02315, N(SI)=2.64002
 DEGREES OF FREEDOM 0
T= 2.052127E+03
 BP(GAS)=61.009565, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.987587, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.748921, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   23 FROM STAGE    3
 H=-8.06062E5, P=1E5, N(C)=1.65008, N(N)=3.6E-4, N(O)=3.71618, N(SI)=2.86785
 DEGREES OF FREEDOM 0
T= 2.083867E+03
 BP(GAS)=67.084737, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.252804, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.485245, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   23 FROM STAGE    4
 H=14197.5, P=1E5, N(C)=0.87921, N(N)=2E-4, N(O)=1.91353, N(SI)=1.83597
 DEGREES OF FREEDOM 0
T= 2.269500E+03
 BP(GAS)=70.264028, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.476822, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   24 FROM STAGE    1
 H=-9.94284E5, P=1E5, N(C)=2.94854, N(N)=6.784E-4, N(O)=3.83371,
    N(SI)=1.68521
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.325561, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=21.335974, BP(CRISTOBALITE)=68.838274, BP(DIAMOND)=0,
    BP(GRAPHITE)=10.589356, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   24 FROM STAGE    2
 H=-9.26367E5, P=1E5, N(C)=2.16234, N(N)=5.18E-4, N(O)=4.02059, N(SI)=2.65869
 DEGREES OF FREEDOM 0
T= 2.054109E+03
 BP(GAS)=61.182133, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.000817, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.790849, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   24 FROM STAGE    3
 H=-8.07308E5, P=1E5, N(C)=1.65111, N(N)=3.6E-4, N(O)=3.72082, N(SI)=2.87127
 DEGREES OF FREEDOM 0
T= 2.083880E+03
 BP(GAS)=67.147679, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
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    BP(C1SI1_BETA)=35.279965, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.578045, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   24 FROM STAGE    4
 H=13011.1, P=1E5, N(C)=0.879887, N(N)=2E-4, N(O)=1.91662, N(SI)=1.8382
 DEGREES OF FREEDOM 0
T= 2.258539E+03
 BP(GAS)=70.385643, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.475169, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   25 FROM STAGE    1
 H=-9.93853E5, P=1E5, N(C)=2.93135, N(N)=6.784E-4, N(O)=3.83093,
    N(SI)=1.69961
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.360421, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=21.993986, BP(CRISTOBALITE)=68.717389, BP(DIAMOND)=0,
    BP(GRAPHITE)=10.170946, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   25 FROM STAGE    2
 H=-9.26049E5, P=1E5, N(C)=2.1443, N(N)=5.18E-4, N(O)=4.01827, N(SI)=2.67439
 DEGREES OF FREEDOM 0
T= 2.055734E+03
 BP(GAS)=61.325484, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.011422, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.824207, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   25 FROM STAGE    3
 H=-8.08257E5, P=1E5, N(C)=1.65192, N(N)=3.6E-4, N(O)=3.7244, N(SI)=2.87392
 DEGREES OF FREEDOM 0
T= 2.083891E+03
 BP(GAS)=67.197432, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.300888, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.648624, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   25 FROM STAGE    4
 H=12109., P=1E5, N(C)=0.880409, N(N)=2E-4, N(O)=1.91897, N(SI)=1.83989
 DEGREES OF FREEDOM 0
T= 2.250176E+03
 BP(GAS)=70.47823, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.474083, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   26 FROM STAGE    1
 H=-9.93484E5, P=1E5, N(C)=2.91678, N(N)=6.784E-4, N(O)=3.82849,
    N(SI)=1.71175
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.387119, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=22.548384, BP(CRISTOBALITE)=68.615573, BP(DIAMOND)=0,
    BP(GRAPHITE)=9.8184387, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   26 FROM STAGE    2
 H=-9.25767E5, P=1E5, N(C)=2.12908, N(N)=5.18E-4, N(O)=4.01622, N(SI)=2.68754
 DEGREES OF FREEDOM 0
T= 2.057064E+03
 BP(GAS)=61.444184, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.019917, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.850777, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   26 FROM STAGE    3
 H=-8.08981E5, P=1E5, N(C)=1.65255, N(N)=3.6E-4, N(O)=3.72717, N(SI)=2.87596
 DEGREES OF FREEDOM 0
T= 2.083898E+03
 BP(GAS)=67.236826, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.316945, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.702307, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   26 FROM STAGE    4
 H=11422.8, P=1E5, N(C)=0.88081, N(N)=2E-4, N(O)=1.92075, N(SI)=1.84119
 DEGREES OF FREEDOM 0
T= 2.243802E+03
 BP(GAS)=70.548706, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.473348, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   27 FROM STAGE    1
 H=-9.93171E5, P=1E5, N(C)=2.90449, N(N)=6.784E-4, N(O)=3.82638,
    N(SI)=1.72193
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.407584, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.013201, BP(CRISTOBALITE)=68.530223, BP(DIAMOND)=0,
    BP(GRAPHITE)=9.5229002, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   27 FROM STAGE    2
 H=-9.25521E5, P=1E5, N(C)=2.11631, N(N)=5.18E-4, N(O)=4.01443, N(SI)=2.69851
 DEGREES OF FREEDOM 0
T= 2.058154E+03
 BP(GAS)=61.542207, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.026721, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.871964, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   27 FROM STAGE    3
 H=-8.09533E5, P=1E5, N(C)=1.65304, N(N)=3.6E-4, N(O)=3.7293, N(SI)=2.87754
 DEGREES OF FREEDOM 0
T= 2.083905E+03
 BP(GAS)=67.268068, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.329239, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
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    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.743144, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   27 FROM STAGE    4
 H=10900.9, P=1E5, N(C)=0.881116, N(N)=2E-4, N(O)=1.92211, N(SI)=1.84217
 DEGREES OF FREEDOM 0
T= 2.238945E+03
 BP(GAS)=70.602347, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.472838, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   28 FROM STAGE    1
 H=-9.92907E5, P=1E5, N(C)=2.89418, N(N)=6.784E-4, N(O)=3.82457,
    N(SI)=1.73042
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.423286, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.401312, BP(CRISTOBALITE)=68.458959, BP(DIAMOND)=0,
    BP(GRAPHITE)=9.2761374, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   28 FROM STAGE    2
 H=-9.25308E5, P=1E5, N(C)=2.10564, N(N)=5.18E-4, N(O)=4.01288, N(SI)=2.70763
 DEGREES OF FREEDOM 0
T= 2.059046E+03
 BP(GAS)=61.622967, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.032171, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.888879, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   28 FROM STAGE    3
 H=-8.09954E5, P=1E5, N(C)=1.65342, N(N)=3.6E-4, N(O)=3.73095, N(SI)=2.87876
 DEGREES OF FREEDOM 0
T= 2.083910E+03
 BP(GAS)=67.29288, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.338637, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.774212, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   28 FROM STAGE    4
 H=10503.9, P=1E5, N(C)=0.881351, N(N)=2E-4, N(O)=1.92315, N(SI)=1.84292
 DEGREES OF FREEDOM 0
T= 2.235247E+03
 BP(GAS)=70.643174, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.472477, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   29 FROM STAGE    1
 H=-9.92684E5, P=1E5, N(C)=2.88557, N(N)=6.784E-4, N(O)=3.82302,
    N(SI)=1.73749
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.435345, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.724241, BP(CRISTOBALITE)=68.399659, BP(DIAMOND)=0,
    BP(GRAPHITE)=9.0708202, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   29 FROM STAGE    2
 H=-9.25125E5, P=1E5, N(C)=2.09675, N(N)=5.18E-4, N(O)=4.01156, N(SI)=2.71519
 DEGREES OF FREEDOM 0
T= 2.059777E+03
 BP(GAS)=61.689367, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.036539, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.902395, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   29 FROM STAGE    3
 H=-8.10275E5, P=1E5, N(C)=1.65372, N(N)=3.6E-4, N(O)=3.73223, N(SI)=2.8797
 DEGREES OF FREEDOM 0
T= 2.083913E+03
 BP(GAS)=67.312611, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.345811, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.797852, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   29 FROM STAGE    4
 H=10201.8, P=1E5, N(C)=0.88153, N(N)=2E-4, N(O)=1.92393, N(SI)=1.8435
 DEGREES OF FREEDOM 0
T= 2.232430E+03
 BP(GAS)=70.674247, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.472217, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   30 FROM STAGE    1
 H=-9.92498E5, P=1E5, N(C)=2.8784, N(N)=6.784E-4, N(O)=3.82172, N(SI)=1.74335
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.444615, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.99212, BP(CRISTOBALITE)=68.350461, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.900504, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   30 FROM STAGE    2
 H=-9.2497E5, P=1E5, N(C)=2.08938, N(N)=5.18E-4, N(O)=4.01043, N(SI)=2.72144
 DEGREES OF FREEDOM 0
T= 2.060375E+03
 BP(GAS)=61.743864, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.040041, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.913208, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   30 FROM STAGE    3
 H=-8.10519E5, P=1E5, N(C)=1.65395, N(N)=3.6E-4, N(O)=3.73322, N(SI)=2.88044
 DEGREES OF FREEDOM 0
T= 2.083916E+03
 BP(GAS)=67.328322, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.351285, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.815841, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   30 FROM STAGE    4
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 H=9971.98, P=1E5, N(C)=0.881666, N(N)=2E-4, N(O)=1.92453, N(SI)=1.84393
 DEGREES OF FREEDOM 0
T= 2.230286E+03
 BP(GAS)=70.697899, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.472028, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   31 FROM STAGE    1
 H=-9.92343E5, P=1E5, N(C)=2.87245, N(N)=6.784E-4, N(O)=3.82061,
    N(SI)=1.74821
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.451748, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.213745, BP(CRISTOBALITE)=68.309748, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.7595952, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   31 FROM STAGE    2
 H=-9.24838E5, P=1E5, N(C)=2.08327, N(N)=5.18E-4, N(O)=4.00947, N(SI)=2.72659
 DEGREES OF FREEDOM 0
T= 2.060864E+03
 BP(GAS)=61.788519, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.04285, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.921863, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   31 FROM STAGE    3
 H=-8.10706E5, P=1E5, N(C)=1.65413, N(N)=3.6E-4, N(O)=3.73399, N(SI)=2.88101
 DEGREES OF FREEDOM 0
T= 2.083919E+03
 BP(GAS)=67.340845, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.355459, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.829531, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   31 FROM STAGE    4
 H=9797.08, P=1E5, N(C)=0.88177, N(N)=2E-4, N(O)=1.92499, N(SI)=1.84426
 DEGREES OF FREEDOM 0
T= 2.228654E+03
 BP(GAS)=70.715902, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471889, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   32 FROM STAGE    1
 H=-9.92213E5, P=1E5, N(C)=2.86752, N(N)=6.784E-4, N(O)=3.81969,
    N(SI)=1.75221
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.457241, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.396675, BP(CRISTOBALITE)=68.276134, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.6432877, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   32 FROM STAGE    2
 H=-9.24728E5, P=1E5, N(C)=2.07822, N(N)=5.18E-4, N(O)=4.00867, N(SI)=2.73083
 DEGREES OF FREEDOM 0
T= 2.061265E+03
 BP(GAS)=61.825057, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.045105, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.928798, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   32 FROM STAGE    3
 H=-8.10849E5, P=1E5, N(C)=1.65427, N(N)=3.6E-4, N(O)=3.73458, N(SI)=2.88145
 DEGREES OF FREEDOM 0
T= 2.083921E+03
 BP(GAS)=67.350836, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.35864, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.83995, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   32 FROM STAGE    4
 H=9663.98, P=1E5, N(C)=0.88185, N(N)=2E-4, N(O)=1.92533, N(SI)=1.84452
 DEGREES OF FREEDOM 0
T= 2.227411E+03
 BP(GAS)=70.729605, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471786, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   33 FROM STAGE    1
 H=-9.92106E5, P=1E5, N(C)=2.86345, N(N)=6.784E-4, N(O)=3.81892,
    N(SI)=1.75551
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.461476, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.547354, BP(CRISTOBALITE)=68.248438, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.5474847, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   33 FROM STAGE    2
 H=-9.24635E5, P=1E5, N(C)=2.07406, N(N)=5.18E-4, N(O)=4.008, N(SI)=2.73432
 DEGREES OF FREEDOM 0
T= 2.061592E+03
 BP(GAS)=61.854916, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.046916, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.934356, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   33 FROM STAGE    3
 H=-8.10958E5, P=1E5, N(C)=1.65438, N(N)=3.6E-4, N(O)=3.73504, N(SI)=2.88179
 DEGREES OF FREEDOM 0
T= 2.083922E+03
 BP(GAS)=67.358815, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.361063, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.84788, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   33 FROM STAGE    4
 H=9562.69, P=1E5, N(C)=0.88191, N(N)=2E-4, N(O)=1.9256, N(SI)=1.84471
 DEGREES OF FREEDOM 0
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T= 2.226466E+03
 BP(GAS)=70.740036, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471709, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   34 FROM STAGE    1
 H=-9.92018E5, P=1E5, N(C)=2.8601, N(N)=6.784E-4, N(O)=3.81828, N(SI)=1.75822
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.464743, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.671238, BP(CRISTOBALITE)=68.225659, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.4687171, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   34 FROM STAGE    2
 H=-9.24557E5, P=1E5, N(C)=2.07064, N(N)=5.18E-4, N(O)=4.00744, N(SI)=2.73718
 DEGREES OF FREEDOM 0
T= 2.061859E+03
 BP(GAS)=61.879288, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.04837, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.938815, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   34 FROM STAGE    3
 H=-8.11041E5, P=1E5, N(C)=1.65446, N(N)=3.6E-4, N(O)=3.7354, N(SI)=2.88206
 DEGREES OF FREEDOM 0
T= 2.083924E+03
 BP(GAS)=67.36519, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.362909, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.853916, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   34 FROM STAGE    4
 H=9485.6, P=1E5, N(C)=0.881956, N(N)=2E-4, N(O)=1.9258, N(SI)=1.84486
 DEGREES OF FREEDOM 0
T= 2.225746E+03
 BP(GAS)=70.747975, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471651, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   35 FROM STAGE    1
 H=-9.91944E5, P=1E5, N(C)=2.85734, N(N)=6.784E-4, N(O)=3.81775,
    N(SI)=1.76044
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.467267, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.772923, BP(CRISTOBALITE)=68.206956, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.404063, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   35 FROM STAGE    2
 H=-9.24493E5, P=1E5, N(C)=2.06783, N(N)=5.18E-4, N(O)=4.00698, N(SI)=2.73952
 DEGREES OF FREEDOM 0
T= 2.062077E+03
 BP(GAS)=61.89916, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.049539, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.942393, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   35 FROM STAGE    3
 H=-8.11105E5, P=1E5, N(C)=1.65453, N(N)=3.6E-4, N(O)=3.73568, N(SI)=2.88226
 DEGREES OF FREEDOM 0
T= 2.083924E+03
 BP(GAS)=67.370289, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.364315, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.85851, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   35 FROM STAGE    4
 H=9426.93, P=1E5, N(C)=0.881991, N(N)=2E-4, N(O)=1.92595, N(SI)=1.84497
 DEGREES OF FREEDOM 0
T= 2.225198E+03
 BP(GAS)=70.754019, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471608, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   36 FROM STAGE    1
 H=-9.91884E5, P=1E5, N(C)=2.85508, N(N)=6.784E-4, N(O)=3.8173, N(SI)=1.76227
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.469217, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.856262, BP(CRISTOBALITE)=68.191622, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.3510729, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   36 FROM STAGE    2
 H=-9.24439E5, P=1E5, N(C)=2.06553, N(N)=5.18E-4, N(O)=4.00659, N(SI)=2.74144
 DEGREES OF FREEDOM 0
T= 2.062255E+03
 BP(GAS)=61.915348, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.050478, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.945266, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   36 FROM STAGE    3
 H=-8.11153E5, P=1E5, N(C)=1.65458, N(N)=3.6E-4, N(O)=3.7359, N(SI)=2.88243
 DEGREES OF FREEDOM 0
T= 2.083925E+03
 BP(GAS)=67.374368, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.365386, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.862006, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   36 FROM STAGE    4
 H=9382.28, P=1E5, N(C)=0.882018, N(N)=2E-4, N(O)=1.92607, N(SI)=1.84505
 DEGREES OF FREEDOM 0
T= 2.224780E+03
 BP(GAS)=70.758618, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
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    BP(SI_L)=22.471575, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   37 FROM STAGE    1
 H=-9.91834E5, P=1E5, N(C)=2.85322, N(N)=6.784E-4, N(O)=3.81694,
    N(SI)=1.76376
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.470726, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.924473, BP(CRISTOBALITE)=68.179066, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.3077016, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   37 FROM STAGE    2
 H=-9.24394E5, P=1E5, N(C)=2.06364, N(N)=5.18E-4, N(O)=4.00627, N(SI)=2.743
 DEGREES OF FREEDOM 0
T= 2.062401E+03
 BP(GAS)=61.928524, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.051234, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.947572, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   37 FROM STAGE    3
 H=-8.11191E5, P=1E5, N(C)=1.65462, N(N)=3.6E-4, N(O)=3.73607, N(SI)=2.88255
 DEGREES OF FREEDOM 0
T= 2.083926E+03
 BP(GAS)=67.377634, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.366201, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.864666, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   37 FROM STAGE    4
 H=9348.31, P=1E5, N(C)=0.882038, N(N)=2E-4, N(O)=1.92616, N(SI)=1.84512
 DEGREES OF FREEDOM 0
T= 2.224463E+03
 BP(GAS)=70.762119, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.47155, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   38 FROM STAGE    1
 H=-9.91794E5, P=1E5, N(C)=2.8517, N(N)=6.784E-4, N(O)=3.81664, N(SI)=1.76498
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.471894, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.980232, BP(CRISTOBALITE)=68.168799, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.2722466, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   38 FROM STAGE    2
 H=-9.24358E5, P=1E5, N(C)=2.0621, N(N)=5.18E-4, N(O)=4.00601, N(SI)=2.74428
 DEGREES OF FREEDOM 0
T= 2.062519E+03
 BP(GAS)=61.939239, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.051841, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.949425, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   38 FROM STAGE    3
 H=-8.11219E5, P=1E5, N(C)=1.65465, N(N)=3.6E-4, N(O)=3.7362, N(SI)=2.88265
 DEGREES OF FREEDOM 0
T= 2.083926E+03
 BP(GAS)=67.38025, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.366821, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.866691, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   38 FROM STAGE    4
 H=9322.46, P=1E5, N(C)=0.882054, N(N)=2E-4, N(O)=1.92623, N(SI)=1.84517
 DEGREES OF FREEDOM 0
T= 2.224222E+03
 BP(GAS)=70.764782, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471532, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   39 FROM STAGE    1
 H=-9.9176E5, P=1E5, N(C)=2.85046, N(N)=6.784E-4, N(O)=3.81639, N(SI)=1.76598
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.472799, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.025761, BP(CRISTOBALITE)=68.160413, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.2432958, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   39 FROM STAGE    2
 H=-9.24327E5, P=1E5, N(C)=2.06084, N(N)=5.18E-4, N(O)=4.00579, N(SI)=2.74533
 DEGREES OF FREEDOM 0
T= 2.062616E+03
 BP(GAS)=61.947946, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.052329, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.950914, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   39 FROM STAGE    3
 H=-8.11241E5, P=1E5, N(C)=1.65467, N(N)=3.6E-4, N(O)=3.73631, N(SI)=2.88273
 DEGREES OF FREEDOM 0
T= 2.083927E+03
 BP(GAS)=67.382345, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.367293, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.868232, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   39 FROM STAGE    4
 H=9302.8, P=1E5, N(C)=0.882065, N(N)=2E-4, N(O)=1.92628, N(SI)=1.8452
 DEGREES OF FREEDOM 0
T= 2.224038E+03
 BP(GAS)=70.766809, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471517, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   40 FROM STAGE    1
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 H=-9.91733E5, P=1E5, N(C)=2.84944, N(N)=6.784E-4, N(O)=3.81619,
    N(SI)=1.76679
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.4735, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.0629, BP(CRISTOBALITE)=68.15357, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.2196802, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   40 FROM STAGE    2
 H=-9.24302E5, P=1E5, N(C)=2.05981, N(N)=5.18E-4, N(O)=4.00561, N(SI)=2.74618
 DEGREES OF FREEDOM 0
T= 2.062694E+03
 BP(GAS)=61.955017, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.052722, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.95211, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   40 FROM STAGE    3
 H=-8.11257E5, P=1E5, N(C)=1.65469, N(N)=3.6E-4, N(O)=3.73639, N(SI)=2.88279
 DEGREES OF FREEDOM 0
T= 2.083927E+03
 BP(GAS)=67.384025, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.367653, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.869403, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   40 FROM STAGE    4
 H=9287.84, P=1E5, N(C)=0.882074, N(N)=2E-4, N(O)=1.92632, N(SI)=1.84523
 DEGREES OF FREEDOM 0
T= 2.223898E+03
 BP(GAS)=70.768351, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471507, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   41 FROM STAGE    1
 H=-9.9171E5, P=1E5, N(C)=2.84862, N(N)=6.784E-4, N(O)=3.81602, N(SI)=1.76745
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.474045, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.093165, BP(CRISTOBALITE)=68.147991, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.2004349, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   41 FROM STAGE    2
 H=-9.24282E5, P=1E5, N(C)=2.05898, N(N)=5.18E-4, N(O)=4.00547, N(SI)=2.74687
 DEGREES OF FREEDOM 0
T= 2.062758E+03
 BP(GAS)=61.960755, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053038, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.953071, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   41 FROM STAGE    3
 H=-8.1127E5, P=1E5, N(C)=1.65471, N(N)=3.6E-4, N(O)=3.73645, N(SI)=2.88283
 DEGREES OF FREEDOM 0
T= 2.083927E+03
 BP(GAS)=67.385371, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.367926, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.870295, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   41 FROM STAGE    4
 H=9276.47, P=1E5, N(C)=0.882081, N(N)=2E-4, N(O)=1.92635, N(SI)=1.84525
 DEGREES OF FREEDOM 0
T= 2.223792E+03
 BP(GAS)=70.769524, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471498, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   42 FROM STAGE    1
 H=-9.91692E5, P=1E5, N(C)=2.84794, N(N)=6.784E-4, N(O)=3.81589,
    N(SI)=1.76799
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.474468, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.117807, BP(CRISTOBALITE)=68.143448, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.1847648, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   42 FROM STAGE    2
 H=-9.24265E5, P=1E5, N(C)=2.05829, N(N)=5.18E-4, N(O)=4.00535, N(SI)=2.74743
 DEGREES OF FREEDOM 0
T= 2.062810E+03
 BP(GAS)=61.96541, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053292, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.953844, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   42 FROM STAGE    3
 H=-8.1128E5, P=1E5, N(C)=1.65472, N(N)=3.6E-4, N(O)=3.7365, N(SI)=2.88287
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.386451, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368134, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.870973, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   42 FROM STAGE    4
 H=9267.82, P=1E5, N(C)=0.882086, N(N)=2E-4, N(O)=1.92637, N(SI)=1.84527
 DEGREES OF FREEDOM 0
T= 2.223711E+03
 BP(GAS)=70.770415, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471492, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   43 FROM STAGE    1
 H=-9.91677E5, P=1E5, N(C)=2.84739, N(N)=6.784E-4, N(O)=3.81578,
    N(SI)=1.76843
 DEGREES OF FREEDOM 0
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T= 1.785827E+03
 BP(GAS)=43.474796, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.137856, BP(CRISTOBALITE)=68.13975, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.1720159, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   43 FROM STAGE    2
 H=-9.24251E5, P=1E5, N(C)=2.05774, N(N)=5.18E-4, N(O)=4.00525, N(SI)=2.74789
 DEGREES OF FREEDOM 0
T= 2.062852E+03
 BP(GAS)=61.969183, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053497, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.954465, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   43 FROM STAGE    3
 H=-8.11287E5, P=1E5, N(C)=1.65473, N(N)=3.6E-4, N(O)=3.73654, N(SI)=2.8829
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.387317, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368292, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.871488, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   43 FROM STAGE    4
 H=9261.25, P=1E5, N(C)=0.88209, N(N)=2E-4, N(O)=1.92638, N(SI)=1.84528
 DEGREES OF FREEDOM 0
T= 2.223650E+03
 BP(GAS)=70.771093, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471487, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   44 FROM STAGE    1
 H=-9.91665E5, P=1E5, N(C)=2.84694, N(N)=6.784E-4, N(O)=3.81569,
    N(SI)=1.76878
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475052, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.154154, BP(CRISTOBALITE)=68.136743, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.1616514, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   44 FROM STAGE    2
 H=-9.2424E5, P=1E5, N(C)=2.05729, N(N)=5.18E-4, N(O)=4.00517, N(SI)=2.74826
 DEGREES OF FREEDOM 0
T= 2.062886E+03
 BP(GAS)=61.972241, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053661, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.954965, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   44 FROM STAGE    3
 H=-8.11293E5, P=1E5, N(C)=1.65474, N(N)=3.6E-4, N(O)=3.73657, N(SI)=2.88292
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.388011, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368412, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.87188, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   44 FROM STAGE    4
 H=9256.25, P=1E5, N(C)=0.882093, N(N)=2E-4, N(O)=1.9264, N(SI)=1.84529
 DEGREES OF FREEDOM 0
T= 2.223603E+03
 BP(GAS)=70.771609, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471484, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   45 FROM STAGE    1
 H=-9.91655E5, P=1E5, N(C)=2.84658, N(N)=6.784E-4, N(O)=3.81561,
    N(SI)=1.76907
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475251, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.167395, BP(CRISTOBALITE)=68.134299, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.1532312, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   45 FROM STAGE    2
 H=-9.24231E5, P=1E5, N(C)=2.05692, N(N)=5.18E-4, N(O)=4.0051, N(SI)=2.74856
 DEGREES OF FREEDOM 0
T= 2.062914E+03
 BP(GAS)=61.974717, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053794, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.955366, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   45 FROM STAGE    3
 H=-8.11297E5, P=1E5, N(C)=1.65474, N(N)=3.6E-4, N(O)=3.73659, N(SI)=2.88294
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.388569, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368503, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.872177, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   45 FROM STAGE    4
 H=9252.46, P=1E5, N(C)=0.882096, N(N)=2E-4, N(O)=1.92641, N(SI)=1.8453
 DEGREES OF FREEDOM 0
T= 2.223568E+03
 BP(GAS)=70.772, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471481, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   46 FROM STAGE    1
 H=-9.91647E5, P=1E5, N(C)=2.84628, N(N)=6.784E-4, N(O)=3.81555,
    N(SI)=1.76931
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475405, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
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    BP(C1SI1_BETA)=25.178145, BP(CRISTOBALITE)=68.132315, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.1463948, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   46 FROM STAGE    2
 H=-9.24223E5, P=1E5, N(C)=2.05662, N(N)=5.18E-4, N(O)=4.00505, N(SI)=2.7488
 DEGREES OF FREEDOM 0
T= 2.062937E+03
 BP(GAS)=61.976721, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.0539, BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0,
    BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
    BP(SIO2_LIQUID)=65.955689, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   46 FROM STAGE    3
 H=-8.113E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73661, N(SI)=2.88295
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.389016, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368572, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.872403, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   46 FROM STAGE    4
 H=9249.57, P=1E5, N(C)=0.882097, N(N)=2E-4, N(O)=1.92642, N(SI)=1.8453
 DEGREES OF FREEDOM 0
T= 2.223541E+03
 BP(GAS)=70.772298, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471479, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   47 FROM STAGE    1
 H=-9.9164E5, P=1E5, N(C)=2.84604, N(N)=6.784E-4, N(O)=3.8155, N(SI)=1.7695
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475526, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.186868, BP(CRISTOBALITE)=68.130704, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.1408477, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   47 FROM STAGE    2
 H=-9.24217E5, P=1E5, N(C)=2.05638, N(N)=5.18E-4, N(O)=4.00501, N(SI)=2.749
 DEGREES OF FREEDOM 0
T= 2.062955E+03
 BP(GAS)=61.978344, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053986, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.955949, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   47 FROM STAGE    3
 H=-8.11303E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73663, N(SI)=2.88296
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.389375, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368625, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.872575, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   47 FROM STAGE    4
 H=9247.39, P=1E5, N(C)=0.882099, N(N)=2E-4, N(O)=1.92642, N(SI)=1.84531
 DEGREES OF FREEDOM 0
T= 2.223520E+03
 BP(GAS)=70.772524, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471478, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   48 FROM STAGE    1
 H=-9.91635E5, P=1E5, N(C)=2.84585, N(N)=6.784E-4, N(O)=3.81546,
    N(SI)=1.76965
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.47562, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.193941, BP(CRISTOBALITE)=68.129398, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.1363492, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   48 FROM STAGE    2
 H=-9.24212E5, P=1E5, N(C)=2.05618, N(N)=5.18E-4, N(O)=4.00497, N(SI)=2.74916
 DEGREES OF FREEDOM 0
T= 2.062970E+03
 BP(GAS)=61.979656, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.054055, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.956158, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   48 FROM STAGE    3
 H=-8.11305E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73664, N(SI)=2.88297
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.389663, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368665, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.872705, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   48 FROM STAGE    4
 H=9245.73, P=1E5, N(C)=0.8821, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84531
 DEGREES OF FREEDOM 0
T= 2.223505E+03
 BP(GAS)=70.772695, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471476, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   49 FROM STAGE    1
 H=-9.91631E5, P=1E5, N(C)=2.84569, N(N)=6.784E-4, N(O)=3.81543,
    N(SI)=1.76978
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475694, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.199675, BP(CRISTOBALITE)=68.128339, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.132703, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
```

```
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    49 FROM STAGE    2
 H=-9.24208E5, P=1E5, N(C)=2.05603, N(N)=5.18E-4, N(O)=4.00494, N(SI)=2.74929
 DEGREES OF FREEDOM 0
T= 2.062982E+03
 BP(GAS)=61.980717, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.054111, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.956325, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    49 FROM STAGE    3
 H=-8.11306E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73665, N(SI)=2.88298
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.389894, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368695, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.872804, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    49 FROM STAGE    4
 H=9244.47, P=1E5, N(C)=0.8821, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84531
 DEGREES OF FREEDOM 0
T= 2.223493E+03
 BP(GAS)=70.772825, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471475, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    50 FROM STAGE    1
 H=-9.91627E5, P=1E5, N(C)=2.84556, N(N)=6.784E-4, N(O)=3.8154, N(SI)=1.76988
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475751, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.204319, BP(CRISTOBALITE)=68.127481, BP(DIAMOND)=0,
    BP(GRAPHITE)=8.129749, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    50 FROM STAGE    2
 H=-9.24205E5, P=1E5, N(C)=2.0559, N(N)=5.18E-4, N(O)=4.00492, N(SI)=2.7494
 DEGREES OF FREEDOM 0
T= 2.062992E+03
 BP(GAS)=61.981574, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.054155, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.95646, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    50 FROM STAGE    3
 H=-8.11307E5, P=1E5, N(C)=1.65476, N(N)=3.6E-4, N(O)=3.73665, N(SI)=2.88298
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.39008, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368718, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
    BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.872879, BP(SI_L)=0, BP(SI_S)=0,
    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    50 FROM STAGE    4
 H=9243.51, P=1E5, N(C)=0.882101, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84532
 DEGREES OF FREEDOM 0
T= 2.223484E+03
 BP(GAS)=70.772924, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
    BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
    BP(SI_L)=22.471475, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
REACTOR: @@ Currently no nice output is provided in this module. Use POLY-3
REACTOR: @@ to list the constitution in each segment
REACTOR: GO P-3
POLY_3: L-E
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =  1004, label A0  , database: SSUB5

 Conditions:
 H=9243.51, P=1E5, N(C)=0.882101, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84532
 DEGREES OF FREEDOM 0

 Temperature   2223.48 K (  1950.33 C),  Pressure  1.000000E+05
 Number of moles of components  4.65405E+00,  Mass in grams  9.32444E+01
 Total Gibbs energy -1.35902E+06,  Enthalpy  9.24351E+03,  Volume  3.56321E-01

 Component               Moles      W-Fraction  Activity   Potential  Ref.stat
 C                       8.8210E-01  1.1363E-01 5.0909E-03 -9.7618E+04 SER
 N                       2.0000E-04  3.0044E-05 8.4815E-09 -3.4359E+05 SER
 O                       1.9264E+00  3.3054E-01 1.4658E-13 -5.4632E+05 SER
 SI                      1.8453E+00  5.5581E-01 1.5640E-03 -1.1944E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 3.8539E+00, Mass 7.0773E+01, Volume fraction 1.0000E+00  Mass fractions:
 O   4.35491E-01  SI  4.14766E-01  C   1.49703E-01  N   3.95829E-05
 Constitution:
 O1SI1  5.41812E-01  C1O2   2.03424E-05  C      2.35255E-10  O2     9.66134E-14
 C1O1   4.57645E-01  O2SI1  1.70445E-06  N1O1   7.37237E-11
 SI     4.69570E-04  C1SI1  3.44134E-09  C3     4.10874E-12
 N2     5.18835E-05  O      9.67006E-10  C2     3.46774E-12

 SI_L                        Status ENTERED     Driving force  0.0000E+00
 Moles 8.0012E-01, Mass 2.2471E+01, Volume fraction 0.0000E+00  Mass fractions:
 SI  1.00000E+00  C   0.00000E+00  O   0.00000E+00  N   0.00000E+00
POLY_3: @@ This equilibrium is valid for the fourth segment. Note it is
POLY_3: @@ identified with number 1004. The other have numbers 1001, 1002 and 1003.
POLY_3: @@ Good luck for future work with this!
POLY_3: go sys
SYS: set-inter
SYS:
```

tcex25

```
About Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex25\tcex25.TCM"SYS: set-echo
SYS: @@ Simulation of steel refining
SYS: @@
SYS: @@
SYS: @@ Raw iron used to produce steel usually has very high carbon and
SYS: @@ silicon content. Oxygen is thus blown into the furnace to burn off
SYS: @@ carbon. Lime (CaO) is added to form a slag with silica, and the slag
SYS: @@ can be removed. Alloying elements, such as Mn, Ni, Cr and V are added
SYS: @@ to produce desired steel. Since the reaction between oxygen and
SYS: @@ carbon will increase the temperature, scrap iron is added in order to
SYS: @@ keep the temperature constant (we assume the furnace is isolated
SYS: @@ and no heat is lost to the environment). This is a typical steel
SYS: @@ refining process.
SYS: @@
SYS: @@ This example simulates blowing oxygen into a liquid steel of one
SYS: @@ metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles
SYS: @@ of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant
SYS: @@ is the way to simulate the isolation of the furnace. The oxygen
SYS: @@ will react with carbon and increase the temperature. After blowing
SYS: @@ a certain amount of oxygen, scrap iron is added to keep the temperature
SYS: @@ constant.
SYS: @@
SYS: set-log ex25,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: @@ In this example we use data from the slag database
TDB_TCFE8: sw slag3
   ... the command in full is SWITCH_DATABASE
 Current database: Fe-containing Slag  v3.2

 FE                      O  DEFINED
 FEOLIQ  REJECTED
TDB_SLAG3: d-sys ca si mn c
   ... the command in full is DEFINE_SYSTEM
 CA                      SI                      MN
 C  DEFINED
TDB_SLAG3: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 GAS:G       :C C2 C3 C4 C5 C60 C1O1 C1O2 C2O1 C3O2 C1SI1 C1SI2 C2SI1
  C5FE1O5 CA CA2 CA1O1 FE FE2 FE1O1 FE1O2 MN MN1O1 MN1O2 O O2 O3 O1SI1 O2SI1
  O2SI2 SI SI2 SI3:
  > The gaseous mixture is handled by the ideal gas model
 FE_LIQUID:L :C CA FE MN O SI:
  > Fe-rich liquid phase (dilute solution for other elements)
 SLAG:L      :A0_01_C00C04_12_SIO2 A0_01_C00C10_23_FE2O3 A0_01_C00C16_11_FEO
  A0_01_C00C22_11_MNO A0_01_C00C27_11_CAO A0_01_C04C10_SIFE
  A0_01_C04C16_SIFE A0_01_C04C22_SIMN A0_01_C04C27_SICA A0_01_C10C16_FEFE
  A0_01_C10C22_FEMN A0_01_C10C27_FECA A0_01_C16C22_FEMN A0_01_C16C27_FECA
  A0_01_C22C27_MNCA:
  > Slag phase handled by Kapoor-Frohberg-Gaye Quasichemical Cell Model
 CAO         :CAO:
  > This is pure CaO_Lime phase [CaO]
 FEO         :FEO:
  > This is pure FeO_Wustite phase [FeO]
 FE2O3       :FE2O3:
  > This is pure Fe2O3_Hematite phase [Fe2O3]
 FE3O4       :FE3O4:
  > This is pure Fe3O4_Magnetite phase [Fe3O4]
 MNO         :MNO:
  > This is pure MnO_Manganosite phase [MnO]
 SIO2_QUARTZ :SIO2:
  > This is pure SiO2_alpha_Quartz phase [SiO2]
 SIO2_BETA_QUARTZ :SIO2:
  > This is pure SiO2_beta_Quartz phase [SiO2]
 SIO2_TRIDYMITE :SIO2:
  > This is pure SiO2_Tridymite phase [SiO2]
 SIO2_CRISTOBALITE :SIO2:
  > This is pure SiO2_Christobalite phase [SiO2]
 CA3O3_SIO2  :CAO:SIO2:
  > This is pure Ca3SiO5 phase [3CaO-SiO2]
 CA2O2_SIO2  :CAO:SIO2:
  > This is pure Ca2SiO4 phase [2CaO-SiO2]
 CA3O3_SI2O4 :CAO:SIO2:
  > This is pure Ca3Si2O7 phase [3CaO-2SiO2]
 CAO_SIO2    :CAO:SIO2:
  > This is pure CaSiO3 phase [CaO-SiO2]
 FE2O2_SIO2  :FEO:SIO2:
  > This is pure Fe2SiO4 phase [2FeO-SiO2]
 MN2O2_SIO2  :MNO:SIO2:
  > This is pure Mn2SiO4 phase [2MnO-SiO2]
 MNO_SIO2    :MNO:SIO2:
  > This is pure MnSiO3 phase [MnO-SiO2]
 GRAPHITE    :C:
TDB_SLAG3: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'SLAG2 (2006): TCS Fe-Containing Slag Database, V2.3, owned and provided
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      by Thermo-Calc Software.'
   'TCMP2 (2009): TCS Materials Processing Database, V2.5, owned and provided
      by Thermo-Calc Software.'
   'Lina Kjellqvist (2012), unpublished assessments of CaO-Fe2O3 quasi-binary
      system'
   'Pingfang Shi (2009), unpublished assessments of Fe3O4-bearing systems. '
   'Pingfang Shi (2006), unpublished assessments of SiO2-bearing systems. '
  -OK-
TDB_SLAG3: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ Assume we have one ton (1e6 gram) liquid steel with a composition
POLY_3: @@ set of 4 w/o C, 2 w/o Si and 1 w/o Mn.
POLY_3: s-c t=1673,p=1e5,b(fe)=1e6,w(c)=.04,w(si)=.02,w(mn)=.01
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2
 DEGREES OF FREEDOM 2
POLY_3:Hit RETURN to continue
POLY_3: @@ To remove Si, add a small amount of top slag consisting of
POLY_3: @@ pure lime (CaO), 5.6 kg equivalent to 100 moles of CaO
POLY_3: s-i-a n(cao)=100
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
    N(O)=100
 DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1277 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG3

 Conditions:
 T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
    N(O)=100
 DEGREES OF FREEDOM 0

 Temperature   1673.00 K (  1399.85 C),  Pressure  1.000000E+05
 Number of moles of components  2.26739E+04,  Mass in grams  1.08130E+06
 Total Gibbs energy -2.19006E+09,  Enthalpy  1.32046E+09,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.6010E+03  4.0000E-02 7.5454E-02 -3.5947E+04 SER
 CA                      1.0000E+02  3.7065E-03 1.4244E-08 -2.5131E+05 SER
 FE                      1.7906E+04  9.2481E-01 7.1047E-04 -1.0084E+05 SER
 MN                      1.9682E+02  1.0000E-02 5.1231E-06 -1.6945E+05 SER
 O                       1.0000E+02  1.4796E-03 6.6380E-17 -5.1817E+05 SER
 SI                      7.7002E+02  2.0000E-02 1.3697E-06 -1.8780E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.2474E+04, Mass 1.0757E+06, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.29634E-01  SI  2.01042E-02  CA  6.94868E-07
 C   4.02085E-02  MN  1.00521E-02  O   2.36693E-07

 CAO                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.9995E+02, Mass 5.6064E+03, Volume fraction 0.0000E+00  Mass fractions:
 CA  7.14696E-01  C   0.00000E+00  FE  0.00000E+00
 O   2.85304E-01  MN  0.00000E+00  SI  0.00000E+00

 CA3O3_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 1.2313E-02, Mass 3.1236E-01, Volume fraction 0.0000E+00  Mass fractions:
 CA  5.26617E-01  SI  1.23010E-01  FE  0.00000E+00
 O   3.50373E-01  C   0.00000E+00  MN  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 CAO                     ENTERED      0.000000E+00    1.999545E+02
 CA3O3_SIO2              ENTERED      0.000000E+00    1.231298E-02
 FE_LIQUID               ENTERED      0.000000E+00    2.247397E+04
 CA2O2_SIO2              ENTERED     -1.474286E-01    0.000000E+00
 GRAPHITE                ENTERED     -1.870471E-01    0.000000E+00
 SLAG                    ENTERED     -3.278734E-01    0.000000E+00
 CA3O3_SI2O4             ENTERED     -4.942106E-01    0.000000E+00
 CAO_SIO2                ENTERED     -1.019253E+00    0.000000E+00
 GAS                     ENTERED     -2.400540E+00    0.000000E+00
 SIO2_TRIDYMITE          ENTERED     -3.604879E+00    0.000000E+00
 SIO2_CRISTOBALITE       ENTERED     -3.605424E+00    0.000000E+00
 SIO2_BETA_QUARTZ        ENTERED     -3.625809E+00    0.000000E+00
 SIO2_QUARTZ             ENTERED     -3.625823E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -3.699744E+00
 MNO_SIO2 MN2O2_SIO2 MNO FE2O2_SIO2 FEO FE3O4 FE2O3
POLY_3:Hit RETURN to continue
POLY_3: @@ The steel bath will be insulated so no heat disappears
POLY_3: @@ while blowing oxygen. This means that the enthalpy of the
POLY_3: @@ system is constant and the temperature may increase. Set these
POLY_3: @@ conditions
POLY_3: s-c h
   ... the command in full is SET_CONDITION
Value /1.32045762E+09/:
POLY_3: s-c t=none
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=100,
    H=1.32046E9
 DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: @@ When we calculate now we should get exactly the same temperature
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
```

```
 Using already calculated grid
     6 ITS,  CPU TIME USED   1 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1673.
POLY_3: @@ Voila! The same equilibrium calculated with different conditions
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG3

 Conditions:
 P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=100,
    H=1.32046E9
 DEGREES OF FREEDOM 0

 Temperature   1673.00 K (  1399.85 C),  Pressure  1.000000E+05
 Number of moles of components  2.26739E+04,  Mass in grams  1.08130E+06
 Total Gibbs energy -2.19006E+09,  Enthalpy  1.32046E+09,  Volume  0.00000E+00

 Component               Moles      W-Fraction  Activity   Potential  Ref.stat
 C                       3.6010E+03  4.0000E-02 7.5454E-02 -3.5947E+04 SER
 CA                      1.0000E+02  3.7065E-03 1.4244E-08 -2.5131E+05 SER
 FE                      1.7906E+04  9.2481E-01 7.1047E-04 -1.0084E+05 SER
 MN                      1.9682E+02  1.0000E-02 5.1231E-06 -1.6945E+05 SER
 O                       1.0000E+02  1.4796E-03 6.6380E-17 -5.1817E+05 SER
 SI                      7.7002E+02  2.0000E-02 1.3697E-06 -1.8780E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.2474E+04, Mass 1.0757E+06, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.29634E-01  SI  2.01042E-02  CA  6.94868E-07
 C   4.02085E-02  MN  1.00521E-02  O   2.36693E-07

 CAO                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.9995E+02, Mass 5.6064E+03, Volume fraction 0.0000E+00  Mass fractions:
 CA  7.14696E-01  C   0.00000E+00  FE  0.00000E+00
 O   2.85304E-01  MN  0.00000E+00  SI  0.00000E+00

 CA3O3_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 1.2313E-02, Mass 3.1236E-01, Volume fraction 0.0000E+00  Mass fractions:
 CA  5.26617E-01  SI  1.23010E-01  FE  0.00000E+00
 O   3.50373E-01  C   0.00000E+00  MN  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Now set the oxygen content as independent variable
POLY_3: @@ and blow up to 2000 moles of O (i.e. 1000 moles of O2 i.e. 22.4 m3)
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: n(o)
Min value /0/: 100
Max value /1/: 2000
Increment /47.5/: 100
POLY_3: save tcex25 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   100.0000
...OK

 Phase Region from   100.0000     for:
     FE_LIQUID
     CA3O3_SIO2
     CAO
 Global check of removing phase at  1.66663E+02
 Calculated     3 equilibria

 Phase Region from    166.663     for:
     FE_LIQUID
     CA3O3_SIO2
 Global check of adding phase at  1.66799E+02
 Calculated     3 equilibria

 Phase Region from    166.799     for:
     FE_LIQUID
     CA2O2_SIO2
     CA3O3_SIO2
 Global check of removing phase at  2.00157E+02
 Calculated     4 equilibria

 Phase Region from    200.157     for:
     FE_LIQUID
     CA2O2_SIO2
 Global check of adding phase at  2.02166E+02
 Calculated     3 equilibria

 Phase Region from    202.166     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  1.00000E+03 .... OK
 Global test at  2.00000E+03 .... OK
 Terminating at    2000.00
 Calculated    21 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex25\tcex
 25.POLY3
POLY_3: @@ Sometimes trouble here, error 1614 means all conditions not fullfilled.
POLY_3: @@ Try to start with more oxygen ...
POLY_3: read tcex25
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c n(o)
   ... the command in full is SET_CONDITION
Value /100/: 200
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          1277 grid points in             0 s
    94 ITS,  CPU TIME USED   1 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG3
```

```
 Conditions:
 P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=200,
    H=1.32046E9
 DEGREES OF FREEDOM 0

 Temperature   1723.42 K (  1450.27 C),  Pressure  1.000000E+05
 Number of moles of components  2.27812E+04,  Mass in grams  1.08302E+06
 Total Gibbs energy -2.34831E+09,  Enthalpy  1.32046E+09,  Volume  0.00000E+00

 Component               Moles      W-Fraction  Activity   Potential  Ref.stat
 C                       3.6068E+03  4.0000E-02 6.5488E-02 -3.9060E+04 SER
 CA                      1.0000E+02  3.7006E-03 1.5356E-09 -2.9081E+05 SER
 FE                      1.7906E+04  9.2334E-01 6.2289E-04 -1.0577E+05 SER
 MN                      1.9713E+02  1.0000E-02 4.3101E-06 -1.7703E+05 SER
 O                       2.0000E+02  2.9545E-03 7.6249E-16 -4.9881E+05 SER
 SI                      7.7124E+02  2.0000E-02 1.2968E-06 -1.9424E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.2431E+04, Mass 1.0744E+06, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.30742E-01  SI  1.88553E-02  O   2.34486E-06
 C   4.03204E-02  MN  1.00801E-02  CA  1.80134E-08

 CA2O2_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 3.4836E+02, Mass 8.5714E+03, Volume fraction 0.0000E+00  Mass fractions:
 CA  4.65382E-01  SI  1.63060E-01  FE  0.00000E+00
 O   3.71558E-01  C   0.00000E+00  MN  0.00000E+00

 CA3O3_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 1.4085E+00, Mass 3.5732E+01, Volume fraction 0.0000E+00  Mass fractions:
 CA  5.26617E-01  SI  1.23010E-01  FE  0.00000E+00
 O   3.50373E-01  C   0.00000E+00  MN  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ if still trouble, add that gas should be stable (gas dissolves all)
POLY_3: @@ by increasing oxygen content
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 CA3O3_SIO2              ENTERED      0.000000E+00    1.408525E+00
 CA2O2_SIO2              ENTERED      0.000000E+00    3.483550E+02
 FE_LIQUID               ENTERED      0.000000E+00    2.243144E+04
 SLAG                    ENTERED     -1.455619E-01    0.000000E+00
 CA3O3_SI2O4             ENTERED     -2.500340E-01    0.000000E+00
 GRAPHITE                ENTERED     -2.698781E-01    0.000000E+00
 CAO                     ENTERED     -4.788199E-01    0.000000E+00
 CAO_SIO2                ENTERED     -6.202161E-01    0.000000E+00
 GAS                     ENTERED     -1.307773E+00    0.000000E+00
 SIO2_TRIDYMITE          ENTERED     -2.566026E+00    0.000000E+00
 SIO2_CRISTOBALITE       ENTERED     -2.566180E+00    0.000000E+00
 SIO2_BETA_QUARTZ        ENTERED     -2.587799E+00    0.000000E+00
 SIO2_QUARTZ             ENTERED     -2.587813E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -2.764555E+00
 MNO_SIO2 MN2O2_SIO2 MNO FE2O2_SIO2 FEO FE3O4 FE2O3
POLY_3: c-st p gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/: 1
POLY_3: s-c n(o)=300
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          1277 grid points in             0 s
    37 ITS,  CPU TIME USED   1 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0   , database: SLAG3

 Conditions:
 P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=300,
    H=1.32046E9
 DEGREES OF FREEDOM 0

 Temperature   1737.41 K (  1464.26 C),  Pressure  1.000000E+05
 Number of moles of components  2.28885E+04,  Mass in grams  1.08474E+06
 Total Gibbs energy -2.42505E+09,  Enthalpy  1.32046E+09,  Volume  1.41396E+01

 Component               Moles      W-Fraction  Activity   Potential  Ref.stat
 C                       3.6125E+03  4.0000E-02 5.9862E-02 -4.0675E+04 SER
 CA                      1.0000E+02  3.6947E-03 1.1359E-11 -3.6405E+05 SER
 FE                      1.7906E+04  9.2188E-01 6.0707E-04 -1.0700E+05 SER
 MN                      1.9745E+02  1.0000E-02 4.1965E-06 -1.7886E+05 SER
 O                       3.0000E+02  4.4248E-03 1.1809E-14 -4.6327E+05 SER
 SI                      7.7247E+02  2.0000E-02 1.2680E-06 -1.9614E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.9576E+02, Mass 2.7425E+03, Volume fraction 1.0000E+00  Mass fractions:
 O   5.71009E-01  MN  3.26864E-04  FE  1.77084E-05
 C   4.28581E-01  SI  6.50792E-05  CA  9.33307E-08
 Constitution:
 C1O1      9.99604E-01  C2O1      3.60024E-11  O2        2.65004E-16
 MN        1.66700E-04  FE1O1     2.16563E-11  C1SI1     1.89897E-16
 C1O2      1.55481E-04  C2SI1     1.24191E-12  FE1O2     1.35522E-17
 O1SI1     6.49233E-05  O         1.07250E-12  CA2       4.52820E-18
 FE        8.88424E-06  CA1O1     1.56195E-13  MN1O2     4.07663E-18
 CA        6.52467E-08  FE2       1.23188E-13  C5        7.36602E-20
 O2SI2     4.12168E-10  C1SI2     3.31148E-14  SI3       6.62708E-20
 O2SI1     2.76336E-10  C         3.19274E-14  C4        3.28485E-20
 SI        2.45777E-10  C3        5.66532E-15  C5FE1O5   8.43862E-25
 MN1O1     7.33238E-11  SI2       7.96419E-16  C60       1.00000E-30
 C3O2      5.29278E-11  C2        6.41588E-16  O3        1.00000E-30

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.2343E+04, Mass 1.0734E+06, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.31632E-01  SI  1.89032E-02  O   3.16069E-05
 C   3.93281E-02  MN  1.01049E-02  CA  8.34231E-13

 CA2O2_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 3.5000E+02, Mass 8.6118E+03, Volume fraction 0.0000E+00  Mass fractions:
 CA  4.65382E-01  SI  1.63060E-01  FE  0.00000E+00
 O   3.71558E-01  C   0.00000E+00  MN  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: save tcex25 y
   ... the command in full is SAVE_WORKSPACES
```

```
 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    300.000
...OK

 Phase Region from    300.000     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  1.10000E+03 .... OK
 Terminating at    2000.00
 Calculated    20 equilibria

 Phase Region from    300.000     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global check of removing phase at  2.02166E+02
 Calculated     3 equilibria

 Phase Region from    202.166     for:
     FE_LIQUID
     CA2O2_SIO2
 Global check of adding phase at  2.00157E+02
 Calculated     3 equilibria

 Phase Region from    200.157     for:
     FE_LIQUID
     CA2O2_SIO2
     CA3O3_SIO2
 Global check of removing phase at  1.66799E+02
 Calculated     4 equilibria

 Phase Region from    166.799     for:
     FE_LIQUID
     CA3O3_SIO2
 Global check of adding phase at  1.66663E+02
 Calculated     3 equilibria

 Phase Region from    166.663     for:
     FE_LIQUID
     CA3O3_SIO2
     CAO
 Terminating at   100.0000
 Calculated     4 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex25\tcex
 25.POLY3
POLY_3:
POLY_3: @@ The calculations up to 2000 moles is saved on file. At this
POLY_3: @@ point we will change the conditions and start adding scrap in
POLY_3: @@ order to keep the temperature constant. However, the current
POLY_3: @@ equilibrium is at 100 moles of O so we must first make an
POLY_3: @@ interactive calculation at 2000 moles.
POLY_3: read tcex25
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c n(o)
   ... the command in full is SET_CONDITION
Value /300/: 2005
POLY_3: @@ We choose the value a little bigger than 2000 moles as otherwise the
POLY_3: @@ upper limit of the previous calculation coinsides with the lower limit of
POLY_3: @@ this calculation and that will cause trouble
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          1277 grid points in             0 s
    30 ITS,  CPU TIME USED   1 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1948.7315
POLY_3: @@ We now want to keep the temperature constant by adding scrap
POLY_3: @@ Set the temperature as condition
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /1948.731454/:
POLY_3:
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1948.73, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
    N(O)=2005, H=1.32046E9
 DEGREES OF FREEDOM -1
POLY_3:Hit RETURN to continue
POLY_3: @@ we have too many conditions. Assuming the scrap is pure iron we can
POLY_3: @@ just release the condition on the amount of fe.
POLY_3: s-c b(fe)
   ... the command in full is SET_CONDITION
Value /1000000/: none
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=2005,
    H=1.32046E9
 DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: @@ It is rather special to have both enthalpy
POLY_3: @@ and temperature set as conditions.
POLY_3: @@ We must change the axis limits
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /N(O)/:
Min value /100/: 2000
Max value /2000/: 4000
Increment /50/: 100
POLY_3: @@ We must not give a save command now as that would destroy the
POLY_3: @@ results from the previous step command.
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
```

```
 No initial equilibrium, using default
 Step will start from axis value    2005.00
...OK

 Phase Region from    2005.00      for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  2.80500E+03 .... OK
 Global check of adding phase at  3.77833E+03
 Calculated    20 equilibria

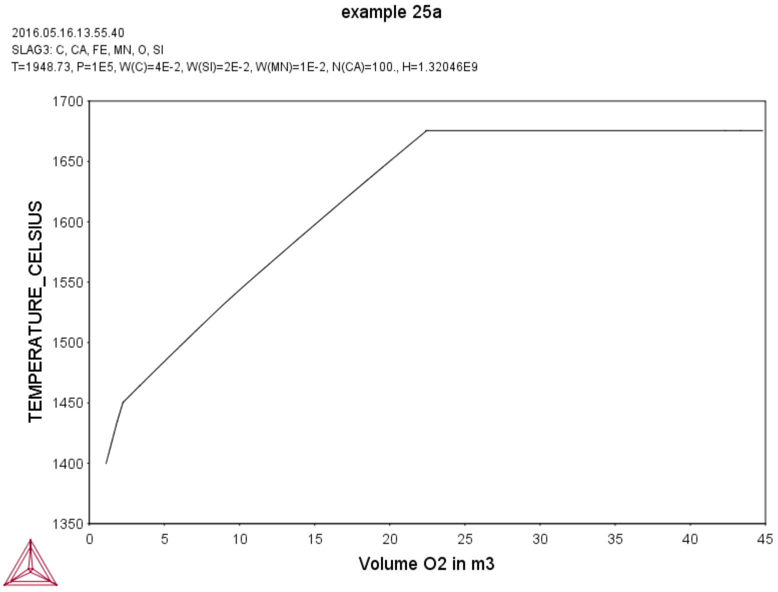
 Phase Region from    3778.33      for:
     GAS
     FE_LIQUID
     SLAG
     CA2O2_SIO2
 Global check of removing phase at  3.87008E+03
 Calculated     4 equilibria

 Phase Region from    3870.08      for:
     GAS
     FE_LIQUID
     SLAG
 Terminating at    4000.00
 Calculated     5 equilibria

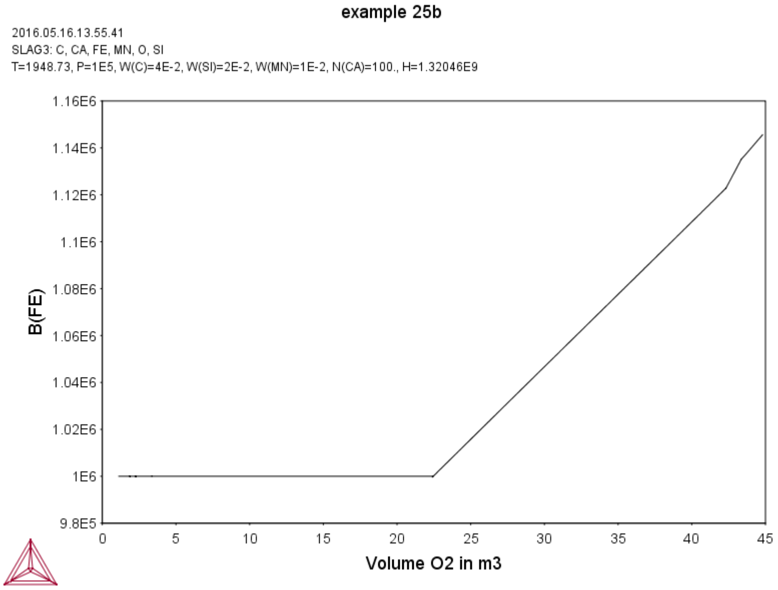
 Phase Region from    2005.00      for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Terminating at    2000.00
 Calculated     4 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex25\tcex
 25.POLY3
POLY_3: @@ We shall now plot the combined results
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

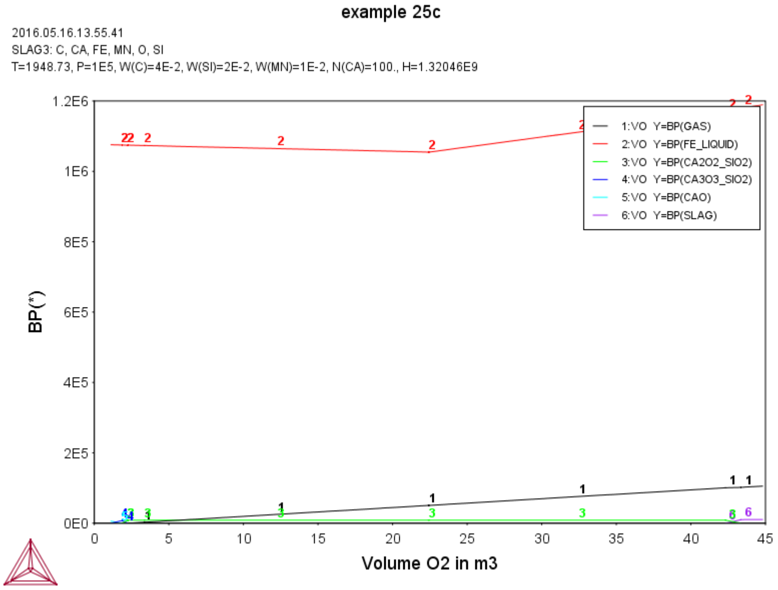
POST: @@ Use volume of added O2 as independent axis, 1 mole O2 is 0.0224 m3
POST: @@ Volume=.0224*(moles of O2)=0.0224*0.5*(moles of O)
POST: enter fun vo=0.0112*n(o);
   ... the command in full is ENTER_SYMBOL
POST: s-d-a x vo
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: @@ Set a nicer axis text
POST: s-a-t-s x n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Volume O2 in m3
POST:
POST:
POST: set-title example 25a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



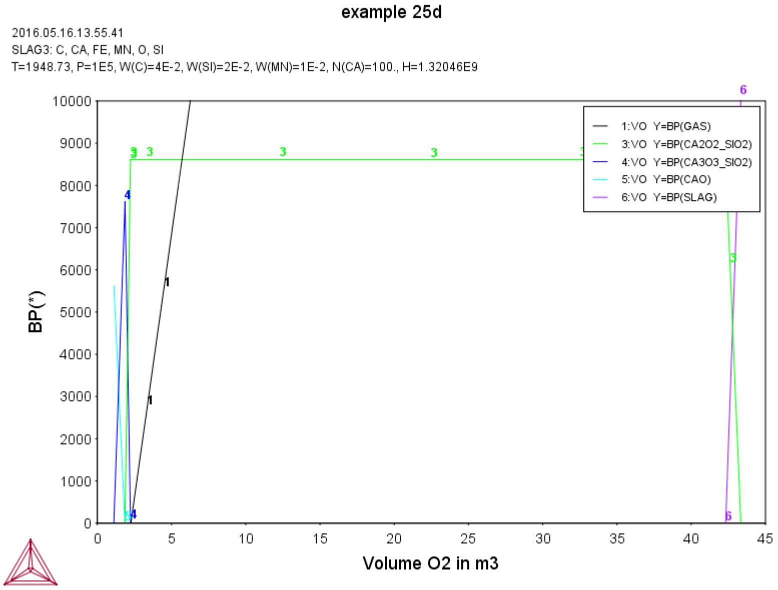
```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the amount of Fe (in grams!)
POST: s-d-a y b(fe)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 25b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



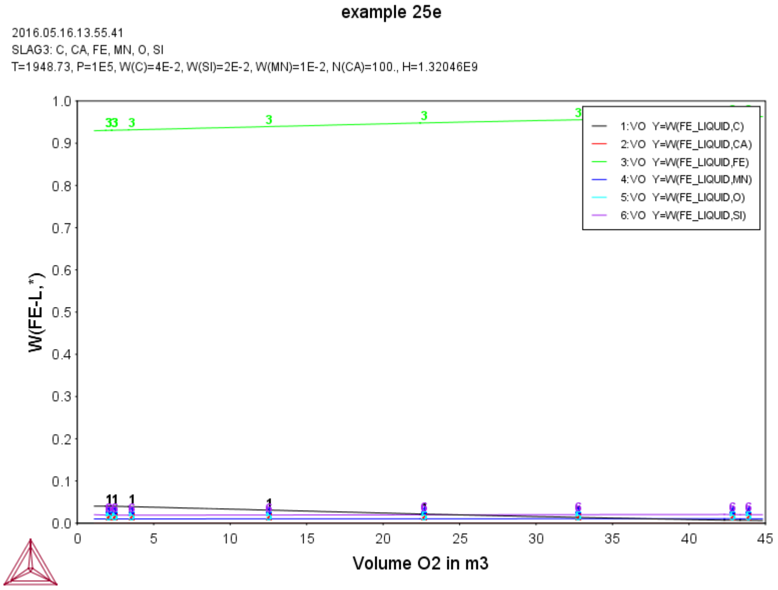
```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the mass of all phases
POST: s-d-a y bp(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: set-lab D
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 25c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



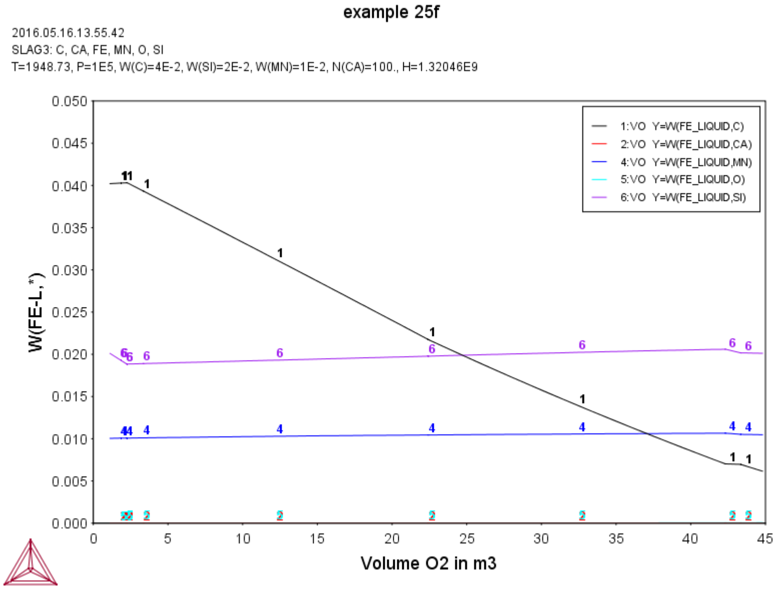
```
POST:
POST:Hit RETURN to continue
POST: @@ Scale up the slag amount.  Liquid slags come at the end only.
POST: s-s y n 0 10000
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 25d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



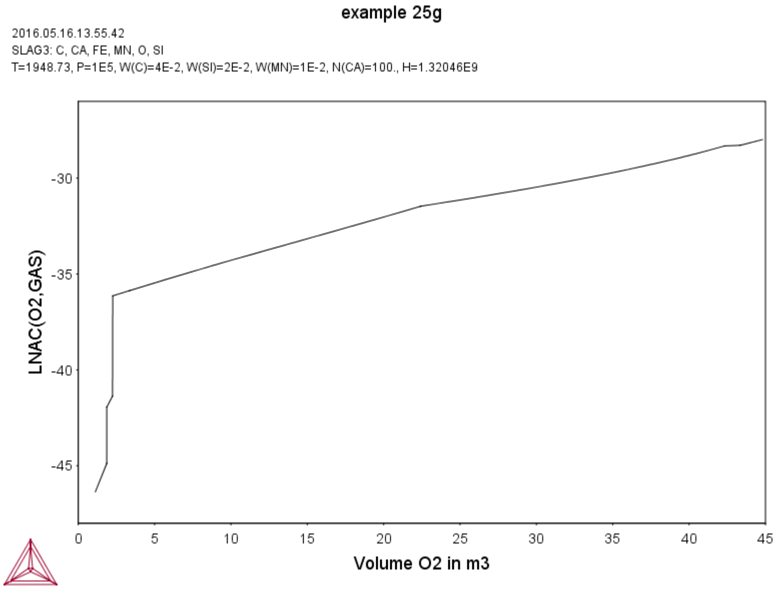
```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot the reason for all this -- the steel composition
POST: s-d-a y w(fe-l,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: set-title example 25e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



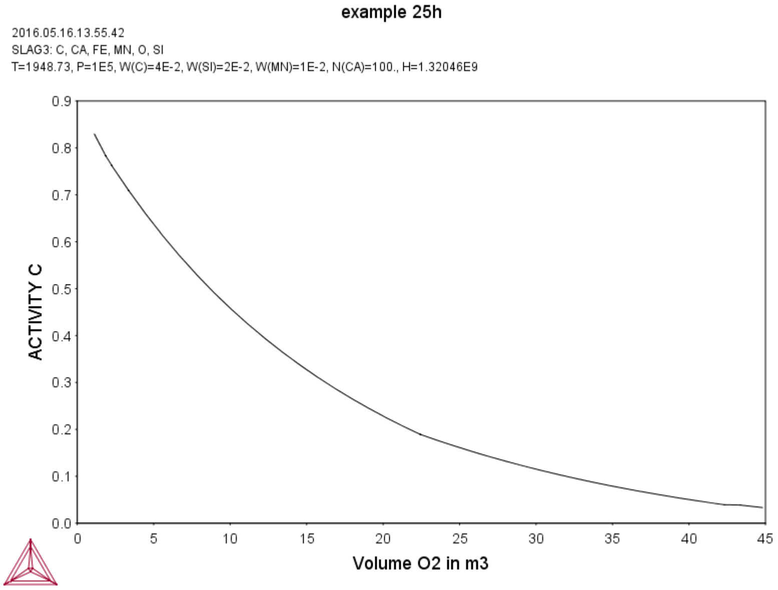
```
POST:
POST:Hit RETURN to continue
POST: @@ Scale up the diagram to get the important part
POST: s-s y n 0 .05
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 25f
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Finally plot the oxygen partial pressure and carbon activity.
POST: @@ For the oxygen plot LN(activity)
POST: s-d-a y lnac(o2,gas)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-lab none
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 25g
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST:
POST: @@ For carbon do not forget to set reference state
POST: set-ref-state c gra * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: s-d-a y ac c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 25h
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex26

```
About Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex26\tcex26.TCM" set-echo
SYS: @@
SYS: @@ Plotting of the partial pressure
SYS: @@ of gas species along the solubility lines
SYS: @@ in the As-Ga Phase diagram
SYS: @@
SYS: @@ Example of plotting the partial pressures of a gas along the
SYS: @@ solubility lines in a phase diagram.
SYS: @@ The system is As-Ga.
SYS: @@ The calculation makes it possible to monitor the input gases to
SYS: @@ a process of depositing solid AsGa
SYS: @@
SYS: set-log ex26,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: @@ At present the data is taken from the special III-V database
TDB_TCFE8: @@ These data will eventually be incorporated in the SGTE solution database
TDB_TCFE8: sw
   ... the command in full is SWITCH_DATABASE
 Use one of these databases

 TCFE8   =  Steels/Fe-Alloys  v8.0
 TCFE9   =  Steels/Fe-Alloys  v9.0 SNAPSHOT
 FROST1  =  FROST database v1.0
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI9   =  Ni-Alloys  v9.0 SNAPSHOT
 TCNI8   =  Ni-Alloys  v8.0
 TCNI7   =  Ni-Alloys  v7.1
 TCNI6   =  Ni-Alloys  v6.0
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.0
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.0 SNAPSHOT
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI1   =  Ti-Alloys  v1.0 SNAPSHOT
 TCCU1   =  Copper  v1.0 SNAPSHOT
 TCCC1   =  Cemented carbide  v1.0
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9f
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB5   =  SGTE Substances Database v5.1
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Nobel Metal Alloys Database v3.1
 SNOB2   =  SGTE Nobel Metal Alloys Database v2.1
 SNOB1   =  SGTE Nobel Metal Alloys Database v1.2
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SNUX6   =  SGTE In-Vessel Nuclear Oxide TDB v6.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.0 snapshot
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX7   =  Metal Oxide Solutions  v7.0 SNAPSHOT
 TCOX6   =  Metal Oxide Solutions  v6.1
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCSLD3  =  Solder Alloys  v3.1
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.0
 TCSI1   =  Ultrapure Silicon  v1.1
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUTO1   =  U-Zr-Si Ternary Oxides TDB v1.1
 NUTA1   =  Ag-Cd-In Ternary Alloys TDB v1.1
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11
 TCAQ2   =  Aqueous Solution  v2.5
 AQS2    =  TGG Aqueous Solution Database v2.5
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 ALDEMO  =  Aluminum Demo Database
 FEDEMO  =  Iron Demo Database
```

```
 NIDEMO  =  Nickel Demo Database
 SLDEMO  =  Solder Demo Database
 OXDEMO  =  Oxide Demo Database
 SUBDEMO =  Substance Demo Database
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 MOB2    =  Alloys Mobility  v2.4
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.0
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBNI4  =  Ni-Alloys Mobility  v4.0
 MOBNI3  =  Ni-Alloys Mobility  v3.1
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0 SNAPSHOT
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database
 MFEDEMO =  Fe-Alloys Mobility demo database
 MNIDEMO =  Ni-Alloys Mobility demo database
 USER    =  User defined Database

DATABASE NAME /TCFE8/: pg35
 Current database: G35 Binary Semi-Conductors TDB v1.2

 VA  DEFINED
 AL1G                    AL2G                    ALASG
 ALPG                    ALP2G                   ALSBG
   REJECTED
 AS1G                    ASGAG                   ASING
 AS2G                    AS3G                    AS4G
   REJECTED
 GA1G                    GA2G                    GAPG
 GASBG                   GASB2G  REJECTED
 IN1G                    IN2G                    INPG
 INSBG                   INSB2G  REJECTED
 P1G                     P2G                     P4G
 SB1G                    SB2G                    SB3G
 SB4G  REJECTED
TDB_PG35: d-sys as ga
   ... the command in full is DEFINE_SYSTEM
 AS                      GA  DEFINED
TDB_PG35: @@ Reject all but the stable phases in this system
TDB_PG35: rej ph /all
   ... the command in full is REJECT
 GAS:G                   LIQUID                  FCC_A1
 HCP_A3                  FCC_B3                  BCT_A5
 BCT_A6                  P_RED                   ASP
 RHOMBO_A7               ORTHO                   GA_GAMMA
   REJECTED
TDB_PG35: rest ph liq rhom ortho fcc_b3 gas:g
   ... the command in full is RESTORE
 LIQUID                  RHOMBO_A7               ORTHO
 FCC_B3                  GAS:G  RESTORED
TDB_PG35: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
 GAS:G       :AS1 AS2 AS3 AS4 AS1GA1 GA1 GA2:
  > Gaseous mixture phase: using the Ideal EOS & Mixing Model
 LIQUID      :AS GA:
  > Liquid mixture phase: Metallic species Al-As-Ga-In-P-Sb
 FCC_B3      :GA:AS:
  > FCC_B3 solution phase: for the complete Al-As-Ga-In-P-Sb system
 RHOMBO_A7   :AS:
  > RHOMBO_A7 solution phase: for the As-Sb binary join only
 ORTHO       :GA:
TDB_PG35:Hit RETURN to continue
TDB_PG35: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'PG35 - ISC Group III-V Binary Simiconductors Database (V1.2), developed
      by Informal cientific Collaboration Group (Ansara I., Chatillon C.,
      Lukas H.L., Nishizawa T., Ohtani H., Ishida K., Hillert M., Sundman B.,
       Argent B.B., Watson A., Chart T. G., and Anderson T.), 1994, as
      published data [A Binary Database for III-V Compound Semiconductor
      Systems, Calphad, 18, 177-222] and provided by Thermo-Calc Software
      (May 2003/June 2008). '
 -OK-
TDB_PG35: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ Set conditions at the As rich side of the system.
POLY_3: @@ We want to calculate the metastable system whithout gas phase
POLY_3: @@ but later plot the gas constitution. Thus set gas to be dormant.
POLY_3: s-c t=1200 p=1e5 n=1 x(ga)=.3
   ... the command in full is SET_CONDITION
POLY_3: c-s p gas=dor
   ... the command in full is CHANGE_STATUS
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           140 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: x
 Output from POLY-3, equilibrium =     1, label A0  , database: PG35
```

```
 Conditions:
 T=1200, P=1E5, N=1, X(GA)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1200.00 K (   926.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  7.33623E+01
 Total Gibbs energy -8.75968E+04,  Enthalpy  1.20850E+04,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 AS                      7.0000E-01  7.0000E-01 1.2211E-03 -6.6929E+04 SER
 GA                      3.0000E-01  3.0000E-01 1.2244E-06 -1.3582E+05 SER

 GAS                         Status DORMANT     Driving force  8.1507E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 AS  1.00000E+00  GA  9.09718E-11
 Constitution:
 AS4     9.80210E-01  AS1     2.30505E-07  GA2     1.87160E-17
 AS2     1.77817E-02  GA1     3.55191E-10
 AS3     2.00768E-03  AS1GA1  5.27773E-12

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.0575E-01, Mass 3.7617E+01, Volume fraction 0.0000E+00  Mole fractions:
 AS  8.95449E-01  GA  1.04551E-01

 FCC_B3                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.9425E-01, Mass 3.5745E+01, Volume fraction 0.0000E+00  Mole fractions:
 AS  5.00000E-01  GA  5.00000E-01
POLY_3:Hit RETURN to continue
POLY_3: @@ Note that the gas would like to be stable (driving force positive)
POLY_3: @@ but it is not allowed to form as it is dormant.
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 LIQUID                  ENTERED      0.000000E+00    5.057539E-01
 FCC_B3                  ENTERED      0.000000E+00    4.942461E-01
 RHOMBO_A7               ENTERED     -4.059045E-01    0.000000E+00
 ORTHO                   ENTERED     -6.644230E+00    0.000000E+00
 GAS                     DORMANT      8.150658E-01
POLY_3: @@ The phase diagram is calculated with the composition and
POLY_3: @@ temperature on the axis as usual
POLY_3: s-a-v 1 x(ga)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 300
Max value /1/: 2000
Increment /42.5/: 25
POLY_3: @@ For an explanation of these symbols see below
POLY_3: ent fun pas1=0.4343*lnacr(as1,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas2=0.4343*lnacr(as2,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas3=0.4343*lnacr(as3,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas4=0.4343*lnacr(as4,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pasga=0.4343*lnacr(as1ga1,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pga1=0.4343*lnacr(ga1,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent tab pp
   ... the command in full is ENTER_SYMBOL
Variable(s): pas1 pas2 pas3 pas4 pasga pga1;
POLY_3:
POLY_3: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED FUNCTIONS AND VARIABLES%
    PAS1=.4343*LNACR(AS1,GAS)
    PAS2=.4343*LNACR(AS2,GAS)
    PAS3=.4343*LNACR(AS3,GAS)
    PAS4=.4343*LNACR(AS4,GAS)
    PASGA=.4343*LNACR(AS1GA1,GAS)
    PGA1=.4343*LNACR(GA1,GAS)
 DEFINED TABLES
    PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
POLY_3:Hit RETURN to continue
POLY_3: ent fun dd=0.4343*dgf(gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas1=log10(y(gas,as1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas2=log10(y(gas,as2))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas3=log10(y(gas,as3))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas4=log10(y(gas,as4))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qasga=log10(y(gas,as1ga1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qga1=log10(y(gas,ga1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent tab qq
   ... the command in full is ENTER_SYMBOL
Variable(s): qas1 qas2 qas3 qas4 qasga qga1;
POLY_3:
POLY_3: ent fun it=1000/T;
   ... the command in full is ENTER_SYMBOL
POLY_3: save tcex26 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED FUNCTIONS AND VARIABLES%
    PAS1=.4343*LNACR(AS1,GAS)
    PAS2=.4343*LNACR(AS2,GAS)
    PAS3=.4343*LNACR(AS3,GAS)
    PAS4=.4343*LNACR(AS4,GAS)
    PASGA=.4343*LNACR(AS1GA1,GAS)
    PGA1=.4343*LNACR(GA1,GAS)
    DD=.4343*DGF(GAS)
    QAS1= LOG10(Y(GAS,AS1) )+DD
    QAS2= LOG10(Y(GAS,AS2) )+DD
```

```
    QAS3= LOG10(Y(GAS,AS3) )+DD
    QAS4= LOG10(Y(GAS,AS4) )+DD
    QASGA= LOG10(Y(GAS,AS1GA1) )+DD
    QGA1= LOG10(Y(GAS,GA1) )+DD
    IT=1000/T
 DEFINED TABLES
    PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
    QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POLY_3:Hit RETURN to continue
POLY_3: @@ Map follows all lines in the phase diagram
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   2.500E-01  3.100E+02
  ** FCC_B3
     RHOMBO_A7
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   2.500E-01  3.000E+02
  ** FCC_B3
     RHOMBO_A7
 Calculated.                     32  equilibria

 Phase region boundary   3 at:   2.500E-01  1.067E+03
  ** FCC_B3
  ** LIQUID
     RHOMBO_A7

 Phase region boundary   4 at:   2.345E-02  1.067E+03
  ** LIQUID
     RHOMBO_A7
 Calculated                     10  equilibria

 Phase region boundary   5 at:   2.734E-01  1.067E+03
     FCC_B3
  ** LIQUID
 Calculated.                    101  equilibria

 Phase region boundary   6 at:   7.500E-01  3.029E+02
     FCC_B3
  ** LIQUID
  ** ORTHO

 Phase region boundary   7 at:   7.500E-01  3.029E+02
     FCC_B3
  ** ORTHO
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   8 at:   1.000E+00  3.029E+02
     LIQUID
  ** ORTHO
 Calculated                     12  equilibria

 Phase region boundary   9 at:   2.500E-01  3.100E+02
  ** FCC_B3
     RHOMBO_A7
 Calculated.                     32  equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   2.500E-01  3.100E+02
  ** FCC_B3
     RHOMBO_A7
 Calculated..                      2  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  11 at:   2.500E-01  3.100E+02
```

```
 ** FCC_B3
    RHOMBO_A7
Calculated.                     32  equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   2.500E-01  3.100E+02
 ** FCC_B3
    RHOMBO_A7
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  13 at:   2.500E-01  3.100E+02
 ** FCC_B3
    RHOMBO_A7
Calculated.                     32  equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                    100  equilibria
Terminating at known equilibrium

Phase region boundary  16 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                    100  equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                    100  equilibria
Terminating at known equilibrium

Phase region boundary  20 at:   2.500E-01  8.700E+02
 ** FCC_B3
    RHOMBO_A7
Calculated..                     24  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  21 at:   2.500E-01  8.700E+02
 ** FCC_B3
    RHOMBO_A7
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   7.492E-01  8.700E+02
 ** FCC_B3
    LIQUID
Calculated.                     24  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.492E-01  8.700E+02
 ** FCC_B3
    LIQUID
Calculated.                     81  equilibria
Terminating at known equilibrium

Phase region boundary  24 at:   3.939E-01  1.430E+03
 ** FCC_B3
    LIQUID
Calculated.                     18  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.939E-01  1.430E+03
 ** FCC_B3
    LIQUID
Calculated.                     87  equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   6.143E-01  1.430E+03
 ** FCC_B3
    LIQUID
Calculated.                     50  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   6.143E-01  1.430E+03
 ** FCC_B3
    LIQUID
Calculated.                     55  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   5.000E-03  1.086E+03
    LIQUID
 ** RHOMBO_A7
Calculated                     15  equilibria

Phase region boundary  29 at:   5.000E-03  1.086E+03
    LIQUID
 ** RHOMBO_A7
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   4.183E-01  1.463E+03
 ** FCC_B3
```

```
    LIQUID
Calculated.                     21  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   4.183E-01  1.463E+03
 ** FCC_B3
    LIQUID
Calculated.                     67  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   5.817E-01  1.468E+03
 ** FCC_B3
    LIQUID
Calculated.                     34  equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   5.817E-01  1.468E+03
 ** FCC_B3
    LIQUID
Calculated.                     54  equilibria
Terminating at known equilibrium

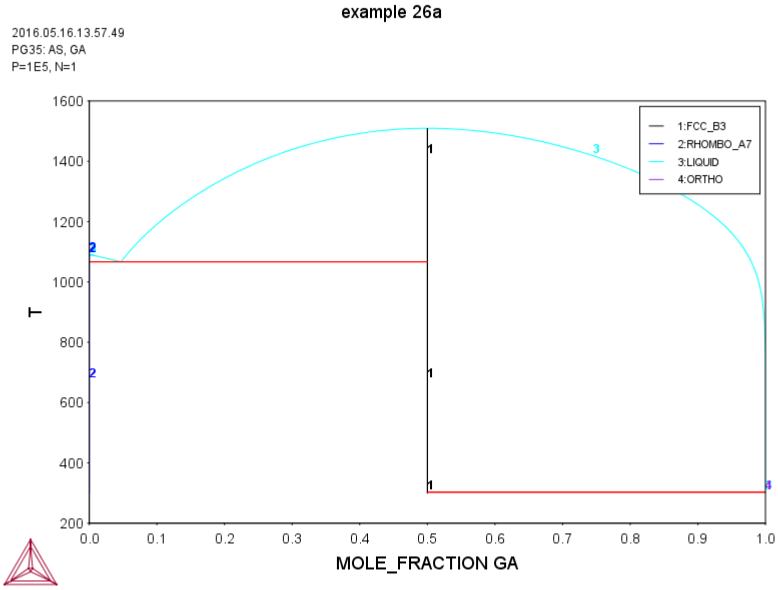
Phase region boundary  34 at:   7.450E-01  9.995E+02
 ** FCC_B3
    LIQUID
Calculated.                     74  equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   7.450E-01  9.995E+02
 ** FCC_B3
    LIQUID
Calculated.                     29  equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex26\tcex
26.POLY3
CPU time for mapping                      0  seconds
POLY_3: @@ Now we plot this in the post processor
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

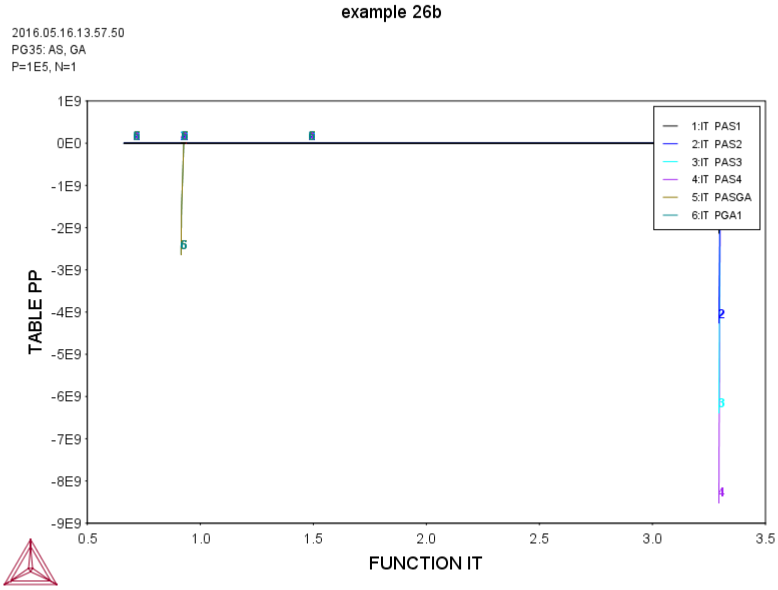

 Setting automatic diagram axes

POST: s-d-a x m-f ga
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 26a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

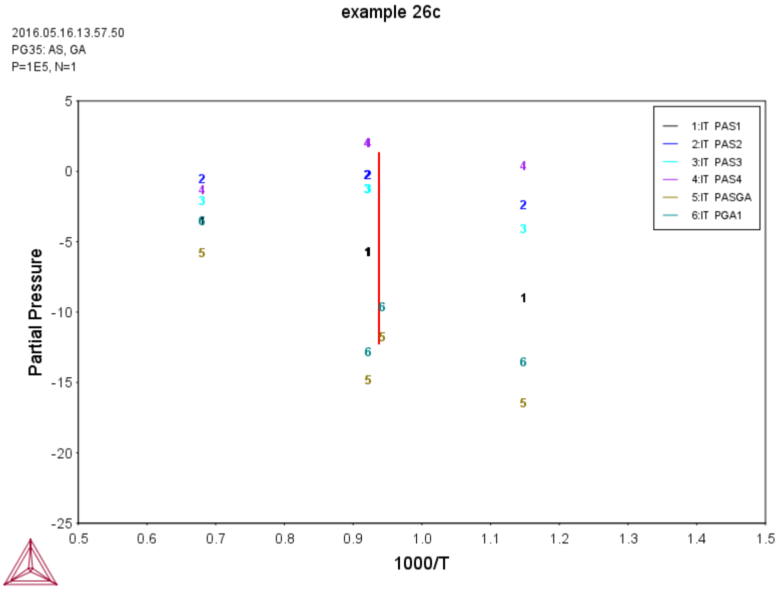


```
POST:
POST:Hit RETURN to continue
POST: @@ This is the traditional phase diagram.
POST: @@
POST: @@ Now those who work with this system is interested to know the
POST: @@ partial pressures of the different gas species along the
POST: @@ solubility lines. As Thermo-Calc saves the complete description of
POST: @@ all tie-lines calculated in a MAP or STEP command, even for
POST: @@ dormat phases, we can now plot these.
POST: @@ The partial pressures of a species in the gas is equal to the
POST: @@ fraction of that species if the gas is stable (Dalton's law)
POST: @@ If the gas is not stable one must add the driving force per
POST: @@ formula unit of the gas (the formula unit depends on the species)
POST: @@
POST: @@ We can obtain directly the activity of a gas species using the
POST: @@ state variable acr(species,gas) which will have as
POST: @@ reference state a pure gas of the species itself. The state variable
POST: @@ lnacr(species,gas) is the natural logarithm of this quantity. To make
POST: @@ it into log10 one must multiply by 0.4343
POST: @@
POST: s-d-a y pp
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: @@ plot againt the inverse of temperature
POST: s-d-a x it
   ... the command in full is SET_DIAGRAM_AXIS
```

```
POST: l-sy
   ... the command in full is LIST_SYMBOLS
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    PAS1=.4343*LNACR(AS1,GAS)
    PAS2=.4343*LNACR(AS2,GAS)
    PAS3=.4343*LNACR(AS3,GAS)
    PAS4=.4343*LNACR(AS4,GAS)
    PASGA=.4343*LNACR(AS1GA1,GAS)
    PGA1=.4343*LNACR(GA1,GAS)
    DD=.4343*DGF(GAS)
    QAS1= LOG10(Y(GAS,AS1) )+DD
    QAS2= LOG10(Y(GAS,AS2) )+DD
    QAS3= LOG10(Y(GAS,AS3) )+DD
    QAS4= LOG10(Y(GAS,AS4) )+DD
    QASGA= LOG10(Y(GAS,AS1GA1) )+DD
    QGA1= LOG10(Y(GAS,GA1) )+DD
    IT=1000/T
    TEMP_C=T-273.15
 DEFINED TABLES
    PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
    QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POST: set-title example 26b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Now make the plot readable by adding axis text and labels
POST: s-s x n 0.5 1.5
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n -25 5
   ... the command in full is SET_SCALING_STATUS
POST: s-a-text x n 1000/T
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-text y n Partial Pressure
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 26c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-interactive
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex27

```
AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex27\tcex27.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example of CVD calculation
SYS: @@
SYS: @@
SYS: @@ Get data from database
SYS: set-log ex27,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw ssub5
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v5.1

 VA  DEFINED
TDB_SSUB5:
TDB_SSUB5: d-sys h cl ar w si
   ... the command in full is DEFINE_SYSTEM
 H                       CL                      AR
 W                       SI  DEFINED
TDB_SSUB5: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   AR1<G> HULTGREN SELECTED VAL 1973 SGTE **
      AR1<G> Ar<G>
      ARGON <GAS>
      STANDARD STATE : CODATA KEY VALUE .
   CL1<G> T.C.R.A.S. Class: 1
      CL1<G> Cl<G>
      CHLORINE <MONATOMIC GAS>
   CL10W2<G> JANAF THERMOCHEMICAL TABLES SGTE
      CL10W2<G> W2Cl10<G>
      TUNGSTEN PENTACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   CL1H1<G> T.C.R.A.S. Class: 1
      CL1H1<G> HCl<G>
      HYDROGEN CHLORIDE <GAS>
   CL1H1SI1<G> T.C.R.A.S. Class: 5
      CL1H1SI1<G> SiHCl<G>
   CL1H3SI1<G> R.W.T.H.-91 SGTE **
      CL1H3SI1<G> SiH3Cl<G>
      MOLWT(G/M): 66.5630
   CL1SI1<G> T.C.R.A.S. Class: 1
      CL1SI1<G> SiCl<G>
      SILICON MONOCHLORIDE <GAS>
   CL1W1<G> T.C.R.A.S. Class: 3
      CL1W1<G> WCl<G>
      TUNGSTEN MONOCHLORIDE <GAS>
   CL2<G> T.C.R.A.S. Class: 1
      CL2<G> Cl2<G> Chlorine gas
      CHLORINE <DIATOMIC GAS>
   CL2H2SI1<G> THERMODATA 01/93
      CL2H2SI1<G> SiH2Cl2<G>
      DICHLOROSILANE
      28/01/93 DICHLOROSILANE.
   CL2SI1<G> T.C.R.A.S. Class: 5
      CL2SI1<G> SiCl2<G>
      SILICON DICHLORIDE <GAS>
   CL2W1<G> JANAF THERMOCHEMICAL TABLES SGT
      CL2W1<G> WCl2<G>
      TUNGSTEN DICHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   CL3H1SI1<G> THERMODATA 01/93
      CL3H1SI1<G> SiHCl3<G>
      28/01/93
   CL3SI1<G> T.C.R.A.S. Class: 6
      CL3SI1<G> SiCl3<G>
      SILICON TRICHLORIDE <GAS>
   CL3W1<G> T.C.R.A.S. Class: 6
      CL3W1<G> WCl3<G>
   CL4SI1<G> T.C.R.A.S. Class: 6
      CL4SI1<G> SiCl4<G>
      SILICON TETRACHLORIDE <GAS>
   CL4W1<G> JANAF THERMOCHEMICAL TABLES SGTE
      CL4W1<G> WCl4<G>
      TUNGSTEN TETRACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   CL5W1<G> JANAF THERMOCHEMICAL TABLES SGTE
      CL5W1<G> WCl5<G>
      TUNGSTEN PENTACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   CL6W1<G> JANAF THERMOCHEMICAL TABLES SGTE
      CL6W1<G> WCl6<G>
      TUNGSTEN HEXACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
      H1<G> H<G>
      HYDROGEN <MONATOMIC GAS>
   H1SI1<G> T.C.R.A.S. Class: 2
      H1SI1<G> SiH<G>
      SILICON MONOHYDRIDE <GAS>
   H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      H2<G> H2<G>
      HYDROGEN<G>
      STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   H2SI1<G> T.C.R.A.S. Class: 6
      H2SI1<G> SiH2<G>
   H3SI1<G> T.C.R.A.S. Class: 5
```

```
      H3SI1<G> SiH3<G>
   H4SI1<G> JANAF 1978; ASSESSMENT DATED 6/76 SGTE
      H4SI1<G> SiH4<G>
      SILANE <GAS>
   H6SI2<G> THERMODATA 01/93
      H6SI2<G> Si2H6<G>
      DISILANE <GAS>
      28/01/93
   SI1<G> T.C.R.A.S. Class: 1
      SI1<G> Si<G>
      SILICON <GAS>
   SI2<G> T.C.R.A.S. Class: 5
      SI2<G> Si2<G>
      SILICON <DIATOMIC GAS>
   SI3<G> T.C.R.A.S. Class: 6
      SI3<G> Si3<G>
      SILICON <TRIATOMIC GAS>
   W1<G> T.C.R.A.S. Class: 4
      W1<G> W<G>
      TUNGSTEN <GAS>
   CL2W1 JANAF THERMOCHEMICAL TABLES SGTE **
      CL2W1 WCl2
      TUNGSTEN DICHLORIDE
      PUBLISHED BY JANAF AT 12/66
      Decomposes and sublimes to complex vapour at about 860K.
   CL3W1 T.C.R.A.S. Class: 7
      CL3W1 WCl3
   CL4SI1<L> N.P.L. SGTE **
      CL4SI1_Liquid SiCl4_Liquid
      SILICON TETRACHLORIDE
      ESTIM.COEF.FOR CP .MELTING PT. AT 203.15 K. LF=1850(#100)CAL/MOL FOR
      GAS
      SEE SI1CL4<G> ABOVE 331 K.
   CL4W1 JANAF THERMOCHEMICAL TABLES SGTE
      CL4W1 WCl4
      TUNGSTEN TETRACHLORIDE
      PUBLISHED BY JANAF AT 12/66
      Decomposes at 771K to WCl2(s) and WCl5(g).
   CL5W1 JANAF THERMOCHEMICAL TABLES SGTE
      CL5W1 WCl5
      TUNGSTEN PENTACHLORIDE
      PUBLISHED BY JANAF AT 12/66
   CL6W1 THERMODATA 01/93
      CL6W1 WCl6
      TUNGSTEN HEXACHLORIDE
      28/01/93 Tb = 613.6 K
   H6SI2 THERMODATA 06/86 BK
      H6SI2 Si2H6
   SI2W1 VAHLAS ET AL **
      SI2W1 WSi2
      from Vahlas et al Calphad 13(3) (1989) 273
   SI3W5 VAHLAS ET AL **
      SI3W5 W5Si3
      from Vahlas et al Calphad 13(3) (1989) 273
   SI1 JANAF THERMOCHEMICAL TABLES SGTE **
      SI1 Si
      SILICON
      PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
      --U.D. 31/10/85
   W1 S.G.T.E. **
      W1 W
      Data from SGTE Unary DB
 -OK-
TDB_SSUB5: @@
TDB_SSUB5: @@ Calculations are made in POLY-3 module
TDB_SSUB5: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@
POLY_3: @@ In poly-3 you define new components
POLY_3: def-com ar cl4w1 cl2h2si1 h2 cl1h1
   ... the command in full is DEFINE_COMPONENTS
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 AR                      ENTERED   SER
 CL4W1                   ENTERED   SER
 CL2H2SI1                ENTERED   SER
 H2                      ENTERED   SER
 CL1H1                   ENTERED   SER
POLY_3:Hit RETURN to continue
POLY_3: @@
POLY_3: @@ Set conditions for input of gases. This may be tricky. The best
POLY_3: @@ is probably to set amounts equal to moles/minutes or something
POLY_3: @@ like that. In this case we had initial partial pressures of
POLY_3: @@ argon 0.9 atm, WCL4 1e-5..0.1 SiH2Cl2 1e-5..0.1 unkown presure of H2.
POLY_3: @@ Should be no addition of HCl nor Cl but added a small addition of
POLY_3: @@ cl1h1 to get equilibrium to converge.
POLY_3: s-c n=1 x(ar)=.9 x(cl2h2si)=1e-3 x(cl4w)=.001 x(cl1h1)=1e-12
   ... the command in full is SET_CONDITION
POLY_3: @@
POLY_3: @@ At the reaction zone T=1000 and total pressure is 1 atm
POLY_3: s-c t=1000 p=101325
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
    P=1.01325E5
 DEGREES OF FREEDOM 0
POLY_3: @@
POLY_3: @@ Save what we have done so far on a file if something happens ...
POLY_3: @@ and then calculate and list the results
POLY_3: save tcex27 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           482 grid points in              0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
```

```
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB5

 Conditions:
 N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
    P=1.01325E5
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  3.65774E+01
 Total Gibbs energy -1.67561E+05,  Enthalpy  1.45855E+04,  Volume  8.21892E-02

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AR                      9.0000E-01  9.8293E-01 2.0867E-09 -1.6619E+05 SER
 CL4W1                   1.0000E-03  8.9034E-03 8.9672E-57 -1.0730E+06 SER
 CL2H2SI1                1.0000E-03  2.7615E-03 1.5207E-40 -7.6231E+05 SER
 H2                      9.8000E-02  5.4008E-03 2.4479E-09 -1.6486E+05 SER
 CL1H1                   1.0021E-12  9.9886E-13 1.9600E-18 -3.3901E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0016E+00, Mass 3.6377E+01, Volume fraction 1.0000E+00  Mass fractions:
 AR        9.88357E-01  CL1H1     5.21203E-03  CL4W1     1.31332E-10
 H2        5.31980E-03  CL2H2SI1  1.11068E-03
 Constitution:
 AR        8.98562E-01  CL        3.03070E-11  H1SI1     1.54528E-17
 H2        9.65533E-02  CL1H1SI1  2.25619E-11  SI        2.70199E-19
 CL1H1     4.48535E-03  CL2W1     1.46463E-11  H6SI2     1.36833E-22
 CL4SI1    3.16220E-04  H4SI1     6.03281E-12  CL5W1     4.37795E-24
 CL3H1SI1  7.81990E-05  CL1SI1    1.41372E-12  SI2       1.26468E-26
 CL1H3SI1  4.29796E-06  CL2       6.15724E-15  CL1W1     1.35601E-30
 CL2H2SI1  3.50040E-07  H3SI1     4.22110E-16  SI3       1.15600E-30
 CL2SI1    2.90182E-07  H2SI1     3.80095E-16  W         1.00000E-30
 CL3SI1    3.29494E-09  CL4W1     1.12601E-16  CL10W2    1.00000E-30
 H         7.01220E-10  CL3W1     1.62069E-17  CL6W1     1.00000E-30

 SI3W5_S                     Status ENTERED     Driving force  0.0000E+00
 Moles-1.6000E-03, Mass 2.0070E-01, Volume fraction 0.0000E+00  Mass fractions:
 CL4W1     1.62262E+00  H2        2.00876E-02  CL1H1    -9.44672E-01
 CL2H2SI1  3.01962E-01  AR        0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Now set axis to vary along the input amounts of WCl4 and SiH2Cl2.
POLY_3: @@ Use logarithmic step as the magnitudes varies a lot.
POLY_3: @@ Note that a limit equal to zero should not be used with log.axis!
POLY_3: s-a-v 1 x(cl2h2si)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1e-8
Max value /1/: 0.02
Increment /4.9999975E-04/: 2.0*
 Logarithmic step set
POLY_3: s-a-v 2 x(cl4w)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1e-8
Max value /1/: 0.02
Increment /4.9999975E-04/: 2.0*
 Logarithmic step set
POLY_3: @@ Add with both direction and continuation ">" to be sure to get all lines
POLY_3: add
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
Direction /Default/: 2>
POLY_3: add -2>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: l-ax
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: X(CL2H2SI1)           Min: 1E-8      Max: 2E-2      Inc: 2*
  Axis No 2: X(CL4W1)              Min: 1E-8      Max: 2E-2      Inc: 2*
POLY_3: li-in
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  +2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
    X(CL1H1)=1.0022937E-12, T=1000, P=101325
 No 2  -2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
    X(CL1H1)=1.0021064E-12, T=1000, P=101325
POLY_3:Hit RETURN to continue
POLY_3: @@
POLY_3: @@ save again with the start point before mapping
POLY_3: save tcex27 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18

 Phase region boundary   1 at:   1.435E-02  1.970E-03
     GAS
     SI2W1_S
  ** SI_S
 Calculated                     68  equilibria

 Phase region boundary   2 at:   1.435E-02  1.970E-03
     GAS
     SI2W1_S
```

```
 ** SI_S
Calculated..                       2  equilibria
Terminating at axis limit.

Phase region boundary   3 at:   2.000E-02  2.810E-03
    GAS
    SI2W1_S
 ** SI_S
Calculated                      70  equilibria

Phase region boundary   4 at:   9.344E-03  1.970E-03
    GAS
    SI2W1_S
 ** SI3W5_S
Calculated                      79  equilibria

Phase region boundary   5 at:   9.344E-03  1.970E-03
    GAS
    SI2W1_S
 ** SI3W5_S
Calculated..                       3  equilibria
Terminating at axis limit.

Phase region boundary   6 at:   2.000E-02  3.793E-03
    GAS
    SI2W1_S
 ** SI3W5_S
Calculated                      84  equilibria

Phase region boundary   7 at:   4.095E-03  1.970E-03
    GAS
 ** SI2W1_S
    SI3W5_S
Calculated                      65  equilibria

Phase region boundary   8 at:   4.095E-03  1.970E-03
    GAS
 ** SI2W1_S
    SI3W5_S
Calculated..                       4  equilibria
Terminating at axis limit.

Phase region boundary   9 at:   2.000E-02  7.114E-03
    GAS
 ** SI2W1_S
    SI3W5_S
Calculated                      70  equilibria

Phase region boundary  10 at:   2.938E-03  1.970E-03
    GAS
    SI3W5_S
 ** W_S
Calculated                      83  equilibria

Phase region boundary  11 at:   2.938E-03  1.970E-03
    GAS
    SI3W5_S
 ** W_S
Calculated..                       4  equilibria
Terminating at axis limit.

Phase region boundary  12 at:   2.000E-02  7.879E-03
    GAS
    SI3W5_S
 ** W_S
Calculated                      84  equilibria

Phase region boundary  13 at:   1.000E-03  1.970E-03
    GAS
 ** SI3W5_S
    W_S
Calculated                      89  equilibria

Phase region boundary  14 at:   1.000E-03  1.970E-03
    GAS
 ** SI3W5_S
    W_S
Calculated..                       6  equilibria
Terminating at axis limit.

Phase region boundary  15 at:   2.000E-02  1.266E-02
    GAS
 ** SI3W5_S
    W_S
Calculated                      99  equilibria

Phase region boundary  16 at:   1.000E-03  1.970E-03
    GAS
 ** SI3W5_S
    W_S
Calculated                      36  equilibria

Phase region boundary  17 at:   1.000E-03  1.970E-03
    GAS
 ** SI3W5_S
    W_S
Calculated..                       7  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   1.000E-03  1.037E-03
    GAS
    SI3W5_S
 ** W_S
Calculated                      35  equilibria

Phase region boundary  19 at:   1.000E-03  1.037E-03
    GAS
    SI3W5_S
 ** W_S
Calculated..                       6  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   1.000E-03  3.753E-04
    GAS
```

```
     SI2W1_S
  ** SI3W5_S
 Calculated                     33  equilibria

 Phase region boundary  21 at:   1.000E-03  3.753E-04
     GAS
     SI2W1_S
  ** SI3W5_S
 Calculated..                      6  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

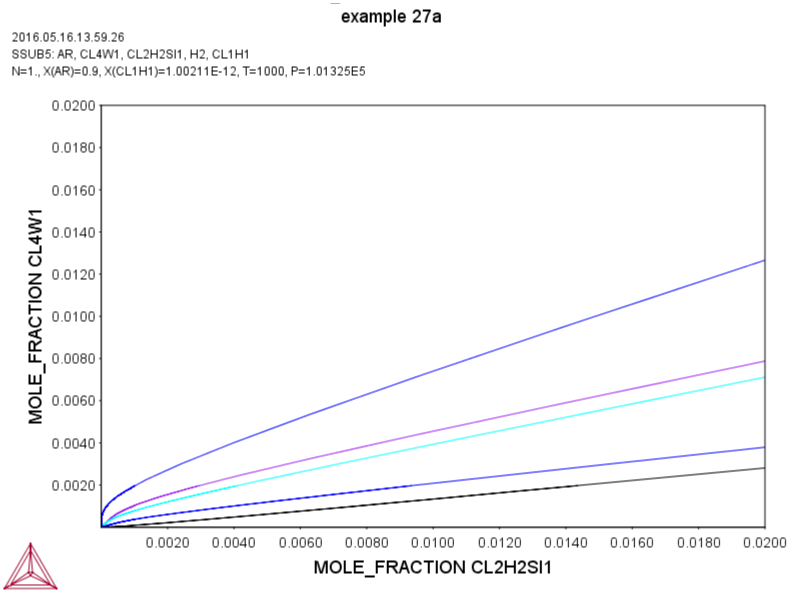
 Phase region boundary  22 at:   1.000E-03  7.855E-04
     GAS
  ** SI2W1_S
     SI3W5_S
 Calculated                     33  equilibria

 Phase region boundary  23 at:   1.000E-03  7.855E-04
     GAS
  ** SI2W1_S
     SI3W5_S
 Calculated..                      6  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex27\tcex
 27.POLY3
 CPU time for mapping                    4  seconds
POLY_3: @@
POLY_3: @@ Plot the diagram in the post processor
POLY_3: post

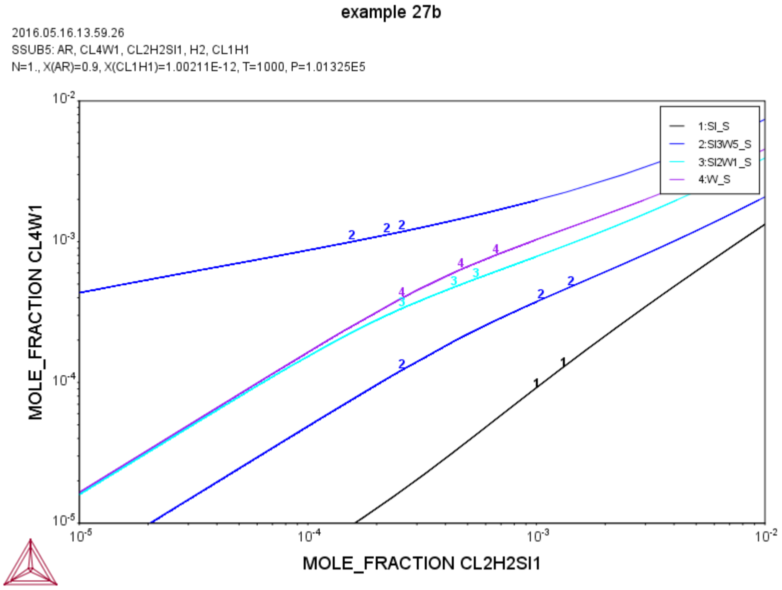
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

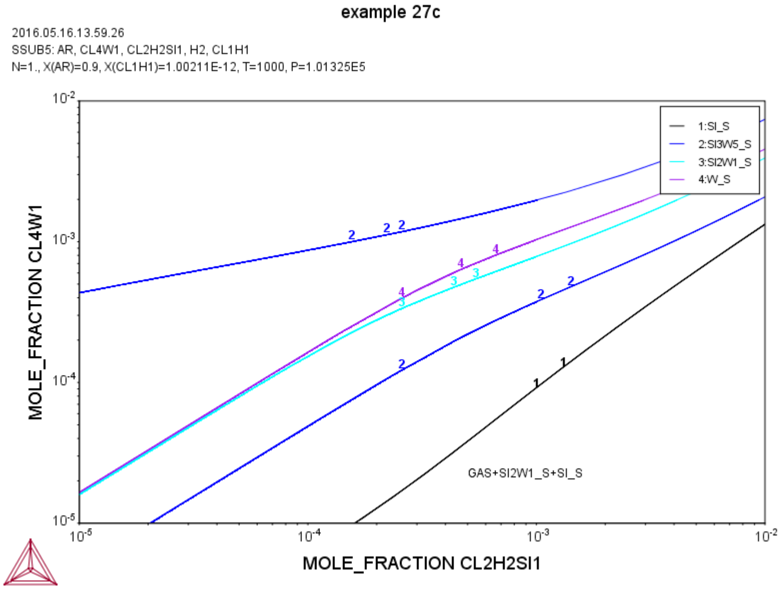
POST:
POST: set-title example 27a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Better with logarithmic axis
POST: s-a-ty x log
   ... the command in full is SET_AXIS_TYPE
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-s x n 1e-5 .01
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 1e-5 .01
   ... the command in full is SET_SCALING_STATUS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: @@
POST: set-title example 27b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@Identify one of the phase regions
POST: add .0005 2e-5
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: GAS+SI2W1_S+SI_S
Text size: /.36/:
POST: set-title example 27c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex28

About

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex28\tcex28.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Example showing calculation of PRE (Pitting Resistance Equivalence)
SYS: @@ for a duplex stainless steel
SYS: @@
SYS: set-log ex28,,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ set the nominal composition
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: cr 25 ni 7 mo 4 c .002 n .27 si .3 mn .3
Next alloying element:
Temperature (C) /1000/: 1050
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MO  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 N  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M6C                      M5C2
 M3C2                     MC_ETA                   MC_SHP
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 Z_PHASE                  FE4N_LP1                 FECN_CHI
 PI                       SIGMA                    MU_PHASE
 P_PHASE                  R_PHASE                  CHI_A12
 LAVES_PHASE_C14          M3SI                     G_PHASE
 CR3SI                    FE2SI                    MSI
 M5SI3                    NBNI3                    NI3TI
 AL4C3                    FE8SI2C                  SIC
 SI3N4                    MN6N4                    MN6N5

Reject phase(s) /NONE/: *
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M6C                     M5C2
 M3C2                    MC_ETA                  MC_SHP
 KSI_CARBIDE             A1_KAPPA                KAPPA
 Z_PHASE                 FE4N_LP1                FECN_CHI
 PI                      SIGMA                   MU_PHASE
 P_PHASE                 R_PHASE                 CHI_A12
 LAVES_PHASE_C14         M3SI                    G_PHASE
 CR3SI                   FE2SI                   MSI
 M5SI3                   NBNI3                   NI3TI
 AL4C3                   FE8SI2C                 SIC
 SI3N4                   MN6N4                   MN6N5
   REJECTED
Restore phase(s):: fcc_a1 bcc_a2 hcp_a3 m23 sigma
 FCC_A1                  BCC_A2                  HCP_A3
 M23C6                   SIGMA  RESTORED
Restore phase(s): /NONE/:

 ........................................................

    The following phases are retained in this system:

 BCC_A2                   FCC_A1                   HCP_A3
 M23C6                    SIGMA

 ........................................................

OK? /Y/:
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....
```

```
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 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated          6136 grid points in             1 s
Found the set of lowest grid points in              0 s
 Creating a new composition set SIGMA#2
 Calculated POLY solution       0 s, total time     1  s
POLY_3:
POLY_3:
POLY_3: save tcex28 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1323.15, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
    W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1323.15 K (  1050.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
```

```
 Total Gibbs energy -7.36372E+04,  Enthalpy  3.91632E+04,  Volume  7.43499E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 2.8934E-05 -1.1497E+05 SER
 CR                      2.6597E-01  2.5000E-01 2.5102E-03 -6.5869E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.6011E-03 -7.0817E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.6138E-06 -1.4142E+05 SER
 MO                      2.3064E-02  4.0000E-02 6.3441E-04 -8.1001E+04 SER
 N                       1.0663E-02  2.7000E-03 4.5323E-07 -1.6070E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.2113E-04 -9.9217E+04 SER
 SI                      5.9088E-03  3.0000E-03 3.2519E-09 -2.1501E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.5763E-01, Mass 3.0640E+01, Volume fraction 5.5307E-01  Mass fractions:
 FE  6.36999E-01  NI  8.57940E-02  N   4.60149E-03  SI  2.58552E-03
 CR  2.34729E-01  MO  3.18218E-02  MN  3.43771E-03  C   3.18713E-05

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.4237E-01, Mass 2.4678E+01, Volume fraction 4.4693E-01  Mass fractions:
 FE  6.24180E-01  NI  5.03909E-02  SI  3.51459E-03  N   3.39204E-04
 CR  2.68960E-01  MO  5.01537E-02  MN  2.45656E-03  C   5.26115E-06
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ Calculate the temperature for equal amount
POLY_3: c-s p bcc_a2=fix .5
   ... the command in full is CHANGE_STATUS
POLY_3: s-c t=none
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          6136 grid points in             1 s
    27 ITS,  CPU TIME USED   1 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1381.4276
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3, W(SI)=3E-3,
    W(MN)=3E-3, P=1E5, N=1
 FIXED PHASES
 BCC_A2=.5
 DEGREES OF FREEDOM 0

 Temperature   1381.43 K (  1108.28 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -7.86534E+04,  Enthalpy  4.13847E+04,  Volume  7.46323E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 2.7951E-05 -1.2043E+05 SER
 CR                      2.6597E-01  2.5000E-01 2.0954E-03 -7.0845E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.3658E-03 -7.5761E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.3755E-06 -1.4875E+05 SER
 MO                      2.3064E-02  4.0000E-02 4.7945E-04 -8.7785E+04 SER
 N                       1.0663E-02  2.7000E-03 6.6471E-07 -1.6337E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.0967E-04 -1.0473E+05 SER
 SI                      5.9088E-03  3.0000E-03 4.7824E-09 -2.2005E+05 SER

 BCC_A2                      Status FIXED       Driving force  0.0000E+00
 Moles 5.0095E-01, Mass 2.7933E+01, Volume fraction 5.0554E-01  Mass fractions:
 FE  6.26660E-01  NI  5.38048E-02  SI  3.46210E-03  N   4.70180E-04
 CR  2.64435E-01  MO  4.86102E-02  MN  2.55179E-03  C   5.96269E-06

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.9905E-01, Mass 2.7385E+01, Volume fraction 4.9446E-01  Mass fractions:
 FE  6.35993E-01  NI  8.65195E-02  N   4.97447E-03  SI  2.52865E-03
 CR  2.35276E-01  MO  3.12173E-02  MN  3.45719E-03  C   3.43184E-05
POLY_3: @@ enter the PRE functions
POLY_3: ent fun prefcc
   ... the command in full is ENTER_SYMBOL
Function: 100*w(fcc_a1,cr)+300*w(fcc_a1,mo)+1600*w(fcc_a1,n);
POLY_3: ent fun prebcc
   ... the command in full is ENTER_SYMBOL
Function: 100*w(bcc_a2,cr)+300*w(bcc_a2,mo)+1600*w(bcc_a2,n);
POLY_3: l-sy
   ... the command in full is LIST_SYMBOLS
 DEFINED FUNCTIONS AND VARIABLES%
    PREFCC=100*W(FCC_A1,CR)+300*W(FCC_A1,MO)+1600*W(FCC_A1,N)
    PREBCC=100*W(BCC_A2,CR)+300*W(BCC_A2,MO)+1600*W(BCC_A2,N)
POLY_3: eval
   ... the command in full is EVALUATE_FUNCTIONS
Name(s): *
 PREFCC=40.851953
 PREBCC=41.778859
POLY_3:Hit RETURN to continue
POLY_3: @@ Now vary the nitrogen content
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(n)
Min value /0/: .001
Max value /1/: .005
Increment /1E-04/: 1E-04
POLY_3: li-ax
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(N)                  Min: 1E-3      Max: 5E-3      Inc: 1E-4
POLY_3: save tcex28 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
 No initial equilibrium, using default
 Step will start from axis value   0.270000E-02
...OK

 Phase Region from   0.270000E-02 for:
     BCC_A2
     FCC_A1
 Global test at  3.50000E-03 .... OK
 Global test at  4.50000E-03 .... OK
 Global test at  4.80000E-03 .... OK
```

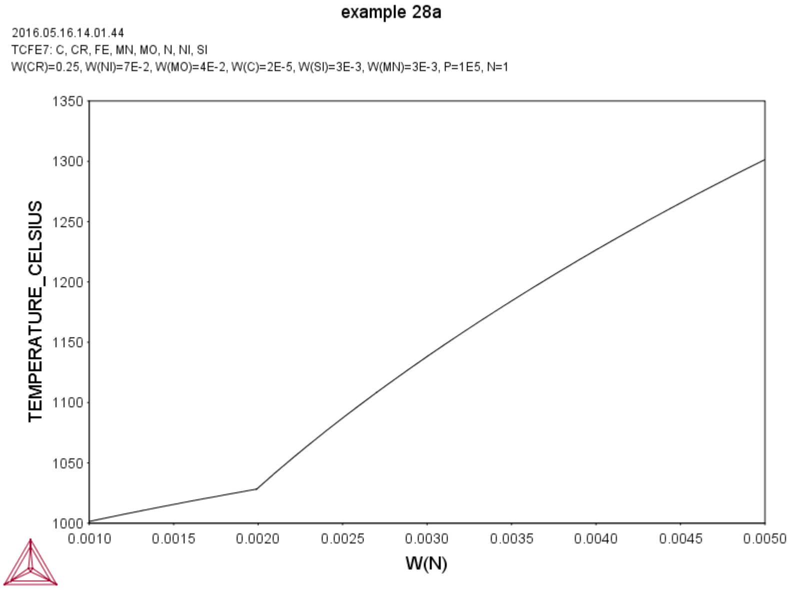
```
 Terminating at   0.500000E-02
 Calculated    26 equilibria

 Phase Region from   0.270000E-02 for:
     BCC_A2
     FCC_A1
 Global check of adding phase at  1.99041E-03
 Calculated    10 equilibria

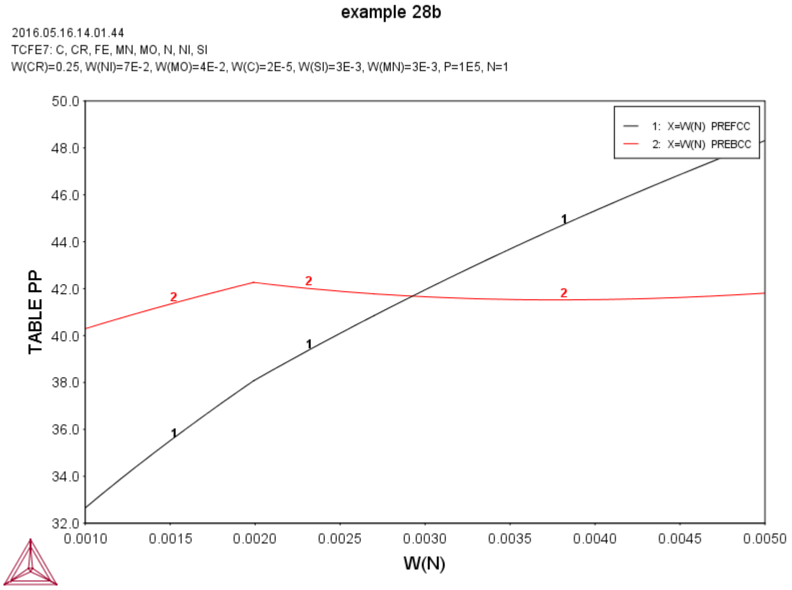
 Phase Region from   0.199041E-02 for:
     BCC_A2
     FCC_A1
     SIGMA
 Global test at  1.20000E-03 .... OK
 Terminating at   0.100000E-02
 Calculated    13 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex28\tcex
 28.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

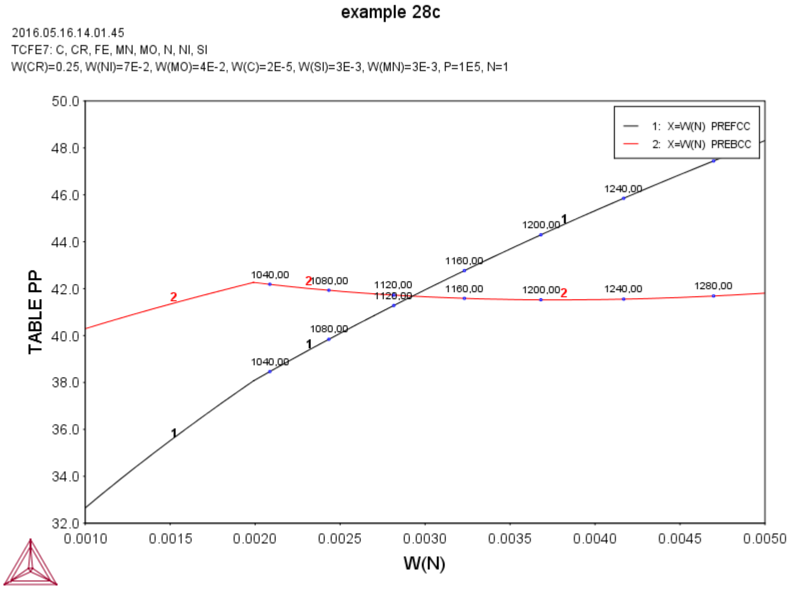
POST:
POST: @@ first plot how the temperature varies
POST: s-d-a x w(n)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 28a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ then plot the PRE
POST: ent tab pp
   ... the command in full is ENTER_SYMBOL
Variable(s): prefcc prebcc
&
POST:
POST: s-d-a y pp
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 28b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ add the temperature as tic marks
POST: s-d-a z t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 800 1300
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 28c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: back
POLY_3: @@ check how close we are to form Cr2N
POLY_3: read tcex28
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: @@ Restore BCC as entered
POLY_3: c-s p bcc_a2=ent 1
   ... the command in full is CHANGE_STATUS
POLY_3: s-c t=1323
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          6136 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
    W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1323.00 K (  1049.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -7.36244E+04,  Enthalpy  3.91576E+04,  Volume  7.43492E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        9.2112E-05  2.0000E-05 2.8937E-05 -1.1496E+05 SER
 CR                       2.6597E-01  2.5000E-01 2.5114E-03 -6.5857E+04 SER
 FE                       6.2530E-01  6.3128E-01 1.6017E-03 -7.0804E+04 SER
 MN                       3.0208E-03  3.0000E-03 2.6144E-06 -1.4140E+05 SER
 MO                       2.3064E-02  4.0000E-02 6.3488E-04 -8.0984E+04 SER
```

```
 N                       1.0663E-02  2.7000E-03 4.5278E-07 -1.6069E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.2117E-04 -9.9203E+04 SER
 SI                      5.9088E-03  3.0000E-03 3.2485E-09 -2.1500E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.5777E-01, Mass 3.0647E+01, Volume fraction 5.5321E-01  Mass fractions:
 FE  6.37001E-01  NI  8.57922E-02  N   4.60067E-03  SI  2.58565E-03
 CR  2.34728E-01  MO  3.18233E-02  MN  3.43767E-03  C   3.18660E-05

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.4223E-01, Mass 2.4671E+01, Volume fraction 4.4679E-01  Mass fractions:
 FE  6.24173E-01  NI  5.03822E-02  SI  3.51472E-03  N   3.38915E-04
 CR  2.68972E-01  MO  5.01574E-02  MN  2.45631E-03  C   5.25959E-06
POLY_3:Hit RETURN to continue
POLY_3: @@ Find out at which temperature sigma will form
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: sigma
 You must release one of these conditions
 T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
 W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
 Testing POLY result by global minimization procedure
Calculated          6136 grid points in             1 s
To form SIGMA the condition is set to T=1305.72281563
POLY_3:Hit RETURN to continue
POLY_3: @@ Find temperature for Cr2N, set start constitution first to
POLY_3: @@ make sure hcp#2 is nitride
POLY_3: s-s-c hcp_a3#2 *
   ... the command in full is SET_START_CONSTITUTION
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: hcp_a3#2
 You must release one of these conditions
 T=1305.72, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
 W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
 Testing POLY result by global minimization procedure
Calculated          6136 grid points in             0 s
To form HCP_A3 the condition is set to T=1254.68882961
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1254.69, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
    W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1254.69 K (   981.54 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -6.78789E+04,  Enthalpy  3.60849E+04,  Volume  7.36619E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 2.9898E-05 -1.0868E+05 SER
 CR                      2.6597E-01  2.5000E-01 3.1144E-03 -6.0211E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.9691E-03 -6.4994E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.9050E-06 -1.3300E+05 SER
 MO                      2.3064E-02  4.0000E-02 6.9498E-04 -7.5859E+04 SER
 N                       1.0663E-02  2.7000E-03 2.7031E-07 -1.5777E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.3051E-04 -9.3306E+04 SER
 SI                      5.9088E-03  3.0000E-03 2.3872E-09 -2.0711E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.2826E-01, Mass 3.9978E+01, Volume fraction 7.2581E-01  Mass fractions:
 FE  6.52952E-01  NI  8.17394E-02  N   3.69563E-03  SI  3.36288E-03
 CR  2.30278E-01  MO  2.45688E-02  MN  3.37715E-03  C   2.69108E-05

 SIGMA                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.4476E-01, Mass 8.2984E+00, Volume fraction 1.4547E-01  Mass fractions:
 FE  5.25243E-01  MO  1.15108E-01  MN  1.74847E-03  C   0.00000E+00
 CR  3.22933E-01  NI  3.48841E-02  SI  8.39239E-05  N   0.00000E+00

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.2697E-01, Mass 7.0417E+00, Volume fraction 1.2872E-01  Mass fractions:
 FE  6.33206E-01  NI  4.47345E-02  SI  4.37633E-03  N   2.29340E-04
 CR  2.76020E-01  MO  3.90957E-02  MN  2.33369E-03  C   4.33440E-06

 HCP_A3#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CR  8.23740E-01  MO  3.89056E-02  NI  1.31664E-03  C   2.52562E-04
 N   1.08069E-01  FE  2.70648E-02  MN  6.51302E-04  SI  2.27285E-08
POLY_3: @@ Rapid cooling needed to avoid these phases!
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3:
```

tcex29

```
About
 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex29\tcex29.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of speciation of a gas
SYS: @@
SYS: set-log ex29,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw ssub5
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v5.1

 VA  DEFINED
TDB_SSUB5:
TDB_SSUB5: d-sys c o h s
   ... the command in full is DEFINE_SYSTEM
 C                       O                       H
 S  DEFINED
TDB_SSUB5: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 GAS:G       :C C1H1 C1H1O1 C1H1O2 C1H2 C1H2O1 C1H2O2_CIS C1H2O2_DIOXIRANE
  C1H2O2_TRANS C1H3 C1H3O1_CH2OH C1H3O1_CH3O C1H4 C1H4O1 C1H4S1 C1O1 C1O1S1
  C1O2 C1S1 C1S2 C2 C2H1 C2H2 C2H2O1 C2H3 C2H4 C2H4O1_ACETALDEHYDE
  C2H4O1_OXIRANE C2H4O2_ACETICACID C2H4O2_DIOXETANE C2H4O3_123TRIOXOLANE
  C2H4O3_124TRIOXOLANE C2H5 C2H6 C2H6O1 C2H6O2 C2O1 C3 C3H1 C3H4_1 C3H4_2
  C3H6_1 C3H6_2 C3H6O1 C3H8 C3O2 C4 C4H1 C4H10_1 C4H10_2 C4H2_1 C4H2_2
  C4H4_1 C4H4_2 C4H6_1 C4H6_2 C4H6_3 C4H6_4 C4H6_5 C4H8_1 C4H8_2 C4H8_3
  C4H8_4 C4H8_5 C4H8_6 C5 C60 C6H6 C6H6O1 H H2 H1O1 H1O2 H2O1 H2O2 H1S1 H2S1
  H2S2 H1O1S1_HSO H1O1S1_SOH H2O1S1_H2SO H2O1S1_HSOH H2O4S1 O O2 O3 O1S1
  O1S2 O2S1 O3S1 S S2 S3 S4 S5 S6 S7 S8:
 GRAPHITE    :C:
 GRAPHITE_L  :C:
 DIAMOND     :C:
 C1H2O2_L    :C1H2O2:
 C1H2S3_L    :C1H2S3:
 C1H4O1_L    :C1H4O1:
 C1H4S1_L    :C1H4S1:
 C1S2_L      :C1S2:
 C2H4O2_L    :C2H4O2:
 C2H6O1_L    :C2H6O1:
 C2H6O2_L    :C2H6O2:
 C60_S       :C60:
 C6H6_L      :C6H6:
 H2O1_L      :H2O1:
 H2O2_L      :H2O2:
 H2S1_L      :H2S1:
 H2S2_L      :H2S2:
 H2O4S1_L    :H2O4S1:
 H4O5S1_L    :H4O5S1:
 H6O6S1_L    :H6O6S1:
 H10O8S1_L   :H10O8S1:
 H15O10_5S1_L :H15O10.5S1:
 H8O7S1_L    :H8O7S1:
 O3S1_L      :O3S1:
 S_S         :S:
 S_S2        :S:
 S_L         :S:
TDB_SSUB5:Hit RETURN to continue
TDB_SSUB5: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
      C1<G> C<G>
   C1H1<G> T.C.R.A.S. Class: 2
      C1H1<G> CH<G>
   C1H1O1<G> T.C.R.A.S. Class: 4
      C1H1O1<G> HCO<G>
      FORMYL <GAS>
   C1H1O2<G> T.C.R.A.S. Class: 6
      C1H1O2<G>
   C1H2<G> T.C.R.A.S. Class: 5
      C1H2<G> CH2<G> METHYLENE
      METHYLENE <GAS>
   C1H2O1<G> T.C.R.A.S. Class: 5
      C1H2O1<G> CH2O<G>
      FORMALDEHYDE <GAS>
   C1H2O2_CIS<G> T.C.R.A.S. Class: 5
      C1H2O2_CIS<G>
   C1H2O2_DIOXIRANE<G> T.C.R.A.S. Class: 6
      C1H2O2_DIOXIRANE<G>
      S298 corrected and cp refitted
      due to corrected data in IVTAN2000 7/2002
   C1H2O2_TRANS<G> T.C.R.A.S. Class: 5
      C1H2O2_TRANS<G>
```

```
C1H3<G> T.C.R.A.S. Class: 5
   C1H3<G> CH3<G>
   METHYL, Gaseous Standard State.
C1H3O1_CH2OH<G> T.C.R.A.S. Class: 6
   C1H3O1_CH2OH<G>
C1H3O1_CH3O<G> T.C.R.A.S. Class: 5
   C1H3O1_CH3O<G>
C1H4<G> T.C.R.A.S. Class: 5
   C1H4<G> CH4<G> METHANE
   METHANE, Gaseous Standard State.
C1H4O1<G> T.C.R.A.S. Class: 5
   C1H4O1<G> CH3OH<G>
   METHANOL <GAS>
C1H4S1<G> THERMODATA 04/98 TC
   C1H4S1<G> METHANETHIOL.
C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
   C1O1<G> CO<G>
   CARBON MONOXIDE <GAS>
   STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
C1O1S1<G> T.C.R.A.S. Class: 2
   C1O1S1<G> COS<G>
   CARBON OXIDE SULFIDE <GAS>
C1O2<G> T.C.R.A.S. Class: 2
   C1O2<G> CO2<G>
   CARBON DIOXIDE <GAS>
C1S1<G> T.C.R.A.S. Class: 1
   C1S1<G> CS<G>
   CARBON MONOSULFIDE <GAS>
C1S2<G> T.C.R.A.S. Class: 3
   C1S2<G> CS2<G>
   CARBON DISULFIDE <GAS>
C2<G> T.C.R.A.S. Class: 2
   C2<G>
   CARBON Diatomic Gas.
C2H1<G> T.C.R.A.S. Class: 6
   C2H1<G> C2H<G>
   CCH RADICAL <GAS>
C2H2<G> T.C.R.A.S. Class: 2
   C2H2<G>
   ACETYLENE (ETYNE). Gaseous Standard State.
C2H2O1<G> T.C.R.A.S. Class: 6
   C2H2O1<G>
   OXIRENE
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C2H3<G> T.C.R.A.S. Class: 6
   C2H3<G>
   DICARBON TRIHYDRIDE, Gaseous Standard State.
C2H4<G> T.C.R.A.S. Class: 6
   C2H4<G>
   ETHYLENE. Gaseous Standard State.
C2H4O1_ACETALDEHYDE<G> T.C.R.A.S. Class: 5
   C2H4O1_ACETALDEHYDE<G>
C2H4O1_OXIRANE<G> T.C.R.A.S. Class: 6
   C2H4O1_OXIRANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C2H4O2_ACETICACID<G> T.C.R.A.S. Class: 5
   C2H4O2_ACETICACID<G>
C2H4O2_DIOXETANE<G> T.C.R.A.S. Class: 6
   C2H4O2_DIOXETANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
   typing error corrected 12/06
C2H4O3_123TRIOXOLANE<G> T.C.R.A.S. Class: 7
   C2H4O3_123TRIOXOLANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C2H4O3_124TRIOXOLANE<G> T.C.R.A.S. Class: 7
   C2H4O3_124TRIOXOLANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
   typing error corrected 12/06
C2H5<G> T.C.R.A.S. Class: 6
   C2H5<G>
   ETHYL radical. Gaseous Standard State.
C2H6<G> T.C.R.A.S. Class: 6
   C2H6<G>
   ETHANE. Gaseous Standard State.
C2H6O1<G> T.C.R.A.S. Class: 6
   C2H6O1<G> C2H6O<G>
   ETHANOL <GAS>
C2H6O2<G> THERMODATA
   C2H6O2<G>
   E-GLYCOL <GAS>.Data revised by THDA.
C2O1<G> T.C.R.A.S. Class: 5
   C2O1<G> C2O<G>
C3<G> T.C.R.A.S. Class: 6
   C3<G>
   CARBON <TRIATOMIC GAS>
C3H1<G> T.C.R.A.S. Class: 6
   C3H1<G> C3H<G>
   2-PROPYNYLIDYNE (gaseous state)
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C3H4_1<G> STULL WESTRUM SINKE 1969 SGTE
   C3H4_1<G>
   ALLENE = 1,2-PROPADIENE (gaseous state)
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H4_2<G> STULL WESTRUM SINKE 1969 SGTE
   C3H4_2<G>
   PROPYNE (METHYLACETYLENE) (gaseous state)
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H6O1<G> THERMODATA 01/93
   C3H6O1<G> ACETONE gas
   ACETONE (gaseous state)
   28/01/93
C3H6_1<G> T.C.R.A.S. Class: 6 4.09.85
   C3H6_1<G> Cyclopropane gas
C3H6_2<G> STULL WESTRUM SINKE 1969 SGTE
   C3H6_2<G> PROPENE gas
   PROPENE (gaseous state)
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H8<G> THERMODATA SGTE
   C3H8<G> PROPANE gas
   PROPANE <Gaseous Standard State>
```

```
C3O2<G> T.C.R.A.S. Class: 6
   C3O2<G>
C4<G> T.C.R.A.S. Class: 7
   C4<G>
C4H1<G> T.C.R.A.S Class: 6
   C4H1<G> C4H<G> 1,3-BUTADIYNYL gas
   1,3-BUTADIYNYL (Gaseous Standard State).
   Data provided by T.C.R.A.S. in 2000
C4H10_1<G> T.C.R.A.S Class: 4
   C4H10_1<G> BUTANE gas
   BUTANE (Gaseous Standard State).
   Data provided by T.C.R.A.S. in 2000
C4H10_2<G> T.C.R.A.S Class: 4
   C4H10_2<G> METHYLPROPANE N-BUTANE gas
   METHYLPROPANE N-BUTANE (Gaseous Standard State).
   Data provided by T.C.R.A.S. in 2000
C4H2_1<G> THERMODATA 1978 ST
   C4H2_1<G> 1,3-BUTADIYNE gas
C4H2_2<G> THERMODATA 06/93 ST
   C4H2_2<G> BUTADIYNE (BIACETYLENE) gas
C4H4_1<G> T.C.R.A.S Class: 6
   C4H4_1<G> 1,3-CYCLOBUTADIENE gas.
   1,3-CYCLOBUTADIENE. Gaseous Standard State.
   Data provided by T.C.R.A.S. in 2000
C4H4_2<G> STULL WESTRUM SINKE 1969 SGTE
   C4H4_2<G> 1-BUTEN-3-YNE VINYLACETYLENE gas
   1-BUTEN-3-YNE VINYLACETYLENE. Gaseous Standard State.
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_1<G> STULL WESTRUM SINKE 1969 SGTE
   C4H6_1<G>
   1,2-BUTADIENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_2<G> STULL WESTRUM SINKE 1969 SGTE
   C4H6_2<G>
   1,3-BUTADIENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_3<G> STULL WESTRUM SINKE 1969 SGTE
   C4H6_3<G>
   1-BUTYNE ETHYLACETYLENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_4<G> STULL WESTRUM SINKE 1969 SGTE
   C4H6_4<G>
   2-BUTYNE DIMETHYLACETYLENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_5<G> T.C.R.A.S Class: 6
   C4H6_5<G>
   CYCLOBUTENE. Data provided by T.C.R.A.S. in 2000
C4H8_1<G> THERMODATA 04/98 TC
   C4H8_1<G> 1-BUTENE gas
C4H8_2<G> THERMODATA 04/98 TC
   C4H8_2<G> (E)-2-BUTENE gas
C4H8_3<G> THERMODATA 04/98 TC
   C4H8_3<G> (Z)-2-BUTENE gas
C4H8_4<G> THERMODATA 04/98 TC
   C4H8_4<G> CYCLOBUTANE gas
C4H8_5<G> THERMODATA 04/98 TC
   C4H8_5<G> 2-METHYLPROPENE gas
C4H8_6<G> THERMODATA 04/98 TC
   C4H8_6<G> METHYLCYCLOPROPANE gas
C5<G> T.C.R.A.S. Class: 7
   C5<G>
C60<G> MHR-95
   C60<G>
   Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
   J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the rotational
   data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that
   a frequency with degeneracy 5 is missing from list in [94Kor/Sid];
   taken to be 419 cm-1, which gives very good, though not exact,
   agreement with values quoted in [94Kor/Sid]. Note discrepancy
   between calculated DrS(298) = -8943.5 J mol K-1 for the reaction
   60C<g>=C60<g>and that given by [94Kor/Sid] in their Table 5,
   -8950 J mol K-1. Enthalpy of formation: DfH = 2588 kJ/mol from
   DsubH(298.15K) = 166 +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure
   values reproduced very well.
   [91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).
C6H6<G> T.C.R.A.S Class: 5
   C6H6<G> BENZENE gas
   BENZENE (Gaseous Standard State).
   Data provided by T.C.R.A.S. in 2000
C6H6O1<G> THERMODATA 01/93
   C6H6O1<G>
   PHENOL gas
   28/01/93
H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
   H1<G> H<G>
   HYDROGEN <MONATOMIC GAS>
H1O1<G> T.C.R.A.S. Class: 1
   H1O1<G> OH<G>
H1O1S1_HSO<G> T.C.R.A.S. Class: 4
   H1O1S1_HSO<G>
H1O1S1_SOH<G> T.C.R.A.S. Class: 5
   H1O1S1_SOH<G>
H1O2<G> T.C.R.A.S. Class: 4
   H1O2<G> HO2<G>
H1S1<G> T.C.R.A.S. Class: 2
   H1S1<G> HS<G>
H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
   H2<G> H2<G>
   HYDROGEN<G>
   STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
H2O1<G> T.C.R.A.S. Class: 1
   H2O1<G> H2O<G>
   WATER <GAS>, STEAM
H2O1S1_H2SO<G> T.C.R.A.S. Class: 4
   H2O1S1_H2SO<G>
H2O1S1_HSOH<G> T.C.R.A.S. Class: 4
   H2O1S1_HSOH<G>
H2O2<G> JANAF SECOND EDIT SGTE
   H2O2<G> H2O2<G>
   HYDROGEN PEROXIDE <GAS>
H2O4S1<G> JANAF 1982; ASSESSMENT DATED 9/77 SGTE
   H2O4S1<G> H2SO4<G>
   SULFURIC ACID <GAS>
H2S1<G> T.C.R.A.S. Class: 2
   H2S1<G> H2S<G>
   HYDROGEN SULFIDE <GAS>
```

```
H2S2<G> K.C. MILLS SGTE **
   H2S2<G> H2S2<G>
   DIHYDROGEN DISULFIDE <GAS>
O1<G> TCRAS 02/06/80
   O1<G> O<G>
O1S1<G> T.C.R.A.S. Class: 3
   O1S1<G> SO<G>
   SULFUR MONOXIDE <GAS>
O1S2<G> JANAF THERMOCHEMICAL TABLES SGTE **
   O1S2<G> S2O<G>
   DISULFUR MONOXIDE <GAS>
   PUBLISHED BY JANAF AT 9/65
O2<G> TCRAS 21/06/90
   O2<G>
   OXYGEN Gaseous Standard State.
O2S1<G> JANAF THERMOCHEMICAL TABLES SGTE **
   O2S1<G> SO2<G>
   SULFUR DIOXIDE <GAS>
   PUBLISHED BY JANAF AT 6/61
O3<G> TCRAS 02/06/80
   O3<G>
   OZONE Gaseous Standard State.
O3S1<G> JANAF THERMOCHEMICAL TABLES SGTE **
   O3S1<G> SO3<G>
   SULFUR TRIOXIDE <GAS>
   PUBLISHED BY JANAF AT 9/65
S1<G> T.C.R.A.S. Class: 1
   S1<G> S<G>
   SULFUR <GAS>
S2<G> T.C.R.A.S. Class: 4
   S2<G> S2<G>
   SULFUR <DIATOMIC GAS>
S3<G> T.C.R.A.S. Class: 5
   S3<G> S3<G>
   SULFUR <3-ATOMIC GAS>
S4<G> T.C.R.A.S. Class: 6
   S4<G> S4<G>
   SULFUR <4-ATOMIC GAS>
S5<G> T.C.R.A.S. Class: 6
   S5<G> S5<G>
   SULFUR <5-ATOMIC GAS>
S6<G> T.C.R.A.S. Class: 6
   S6<G> S6<G>
   SULFUR <6-ATOMIC GAS>
S7<G> T.C.R.A.S. Class: 7
   S7<G> S7<G>
   SULFUR <7-ATOMIC GAS>
S8<G> T.C.R.A.S. Class: 7
   S8<G> S8<G>
   SULFUR <OCTATOMIC GAS>
C1H2O2<L> THERMODATA 01/93
   C1H2O2_Liquid HCOOH_Liquid
   FORMIC ACID MONOMERIC
   28/01/93
C1H2S3<L> THERMODATA 01/86 BC
   C1H2S3_Liquid H2C1S2_Liquid
C1H4O1<L> I. BARIN 3rd. Edition
   C1H4O1_Liquid CH3OH_Liquid
   METHANOL (Liquid). H298 and S298 modified.
C1H4S1<L> THERMODATA 04/99 HH
   C1H4S1<L> METHANETHIOL.
C1S2<L> KUBASCHEWSKI EVANS ALCOCK 1967 SGTE
   C1S2 CS2
   CARBON DISULFIDE
   C1S2 MELTS AT 161.15K LF=1.05(0.1)KCAL/MOLE
C2H4O2<L> THERMODATA 01/93
   C2H4O2_Liquid
   ACETIC ACID (Liquid)
   28/01/93 Tb=389K.
C2H6O1<L> THERMODATA 01/93
   C2H6O1_Liquid C2H6O_Liquid
   ETHANOL (Liquid)
   28/01/93
C2H6O2<L> THERMODATA
   C2H6O2_Liquid
   E-GLYCOL (Liquid)
   Data revised by THDA.
C60 MHR-95
   C60
   Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.
   The
   Fitted to the data in [94Kor/Sid], who took the phase transition at
   257K
   that [94Kor/Sid] do not give an explicit value for S(298.15K).
   S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =425.8 and Cp
   e
   calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]
   in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.
   Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
   the value preferred, if obliquely, by [94Kor/Sid].
   [92Ste/Chi]W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,
   P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).
C6H6<L> THERMODATA 04/99 BC
   C6H6_Liquid BENZENE Liquid
C1<DIAMOND> S.G.T.E. **
   C_DIAMOND
   <DIAMOND>
   Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
   from 1994 database (ex THERMODATA 01/93)
C1<GRAPHITE> S.G.T.E. **
   C_GRAPHITE
   Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
H10O8S1<L> THERMODATA 01/93
   H10O8S1_Liquid H2SO4-4H2O_Liquid
   SULFURIC ACID TETRAHYDRATE.
   28/01/93
H15O10.5S1<L> THERMODATA 01/93
   H15O10.5S1_Liquid H2SO4-6.5H2O_Liquid
   SULFURIC ACID HEMIHEXAHYDRATE.
   28/01/93
H2O1<L> T.C.R.A.S. Class: 4
   H2O1_Liquid H2O_Liquid Pure_Water
   WATER
   T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002
H2O2<L> THERMODATA 01/93
   H2O2_Liquid H2O2_Liquid
```

```
      HYDROGEN PEROXIDE
      28/01/93
   H2O4S1<L> THERMODATA 01/93
      H2O4S1_Liquid H2SO4_Liquid
      SULFURIC ACID
      28/01/93 Tb = 553K.
      S298 modified by NPL 24/11/94. Negative value in Thermodata.
   H2S1<L> THERMODATA 12/94 KK
      H2S1_Liquid H2S_Liquid
   H2S2<L> THERMODATA 11/99 KK
      H2S2_Liquid H2S2_Liquid
   H4O5S1<L> THERMODATA 01/93
      H4O5S1_Liquid H2SO4-H2O_Liquid
      SULFURIC ACID MONOHYDRATE.
      28/01/93
   H6O6S1<L> THERMODATA 01/93
      H6O6S1_Liquid H2SO4-2H2O_Liquid
      H2SO4-2H2O
      28/01/93
   H8O7S1<L> Janaf 4th. Edition
      H8O7S1_Liquid H2SO4-3H2O_Liquid
      SULFURIC ACID TRIHYDRATE
   O3S1<L> THERMODATA 12/94 KK
      O3S1_Liquid SO3_Liquid
   S1 T.C.R.A.S Class: 5
      S1 S
      Data provided by T.C.R.A.S. October 1994.
      Data refitted by I.A.
 -OK-
TDB_SSUB5: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 C                        ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 S                        ENTERED   SER
POLY_3: s-i-a n(h2)=10
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(H)=20
 DEGREES OF FREEDOM 5
POLY_3: s-i-a n(c1o2)=5
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-i-a n(o2s1)=0.1
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1
 DEGREES OF FREEDOM 2
POLY_3: s-c t=1000 p=1e5
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           125 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB5

 Conditions:
 N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1, T=1000, P=1E5
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  3.53000E+01,  Mass in grams  2.46609E+02
 Total Gibbs energy -4.82824E+06,  Enthalpy -1.54921E+06,  Volume  1.23971E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        5.0000E+00  2.4352E-01 3.4847E-02 -2.7910E+04 SER
 H                        2.0000E+01  8.1741E-02 1.0525E-04 -7.6154E+04 SER
 O                        1.0200E+01  6.6173E-01 7.2141E-17 -3.0903E+05 SER
 S                        1.0000E-01  1.3003E-02 9.1466E-08 -1.3476E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 3.5300E+01, Mass 2.4661E+02, Volume fraction 1.0000E+00  Mass fractions:
 O  6.61734E-01  C  2.43523E-01  H  8.17406E-02  S  1.30027E-02
 Constitution:
 H2           4.42736E-01  C3H6_2       1.11399E-13  C4H4_2       3.35580E-21
 H2O1         2.15350E-01  H1O1S1_SOH   3.35036E-14  C4H8_6       1.82465E-21
 C1O1         1.95778E-01  C2H6O1       2.98678E-14  O2           1.76901E-21
 C1O2         1.36417E-01  C2H5         2.60816E-14  C2O1         1.66878E-21
 H2S1         6.57218E-03  C3H8         1.55219E-14  S5           8.95084E-22
 C1H4         3.01187E-03  C1H3O1_CH2OH 7.69302E-15  C2H2O1       5.16353E-22
 C1O1S1       1.34465E-04  H2O1S1_H2SO  2.59570E-15  C4H6_5       3.26857E-22
 H1S1         5.08063E-08  C3H6O1       1.36487E-15  C4H8_4       5.15316E-23
 C1H2O1       4.89873E-08  C2H3         1.30277E-15  H2O4S1       1.59729E-23
 C1H2O2_CIS   4.46604E-08  C3H4_2       1.28184E-15  C4H2_1       8.50232E-24
 H2S2         3.75745E-08  C3O2         7.11139E-16  C4H2_2       8.48033E-24
 C1S2         1.41821E-08  C3H4_1       3.44164E-16  C6H6O1       6.55562E-24
 S2           1.10500E-08  H1O1S1_HSO   1.08974E-16  H1O2         1.72311E-24
 C1H2O2_TRANS 6.42811E-09  C3H6_1       5.22179E-17  C2H1         3.18714E-25
 C2H6         3.64609E-09  C1H3O1_CH3O  1.80849E-17  S6           2.65463E-26
 C2H4         3.02667E-09  C2H4O1_OXIRA 2.11511E-18  C1H1         5.08634E-27
 H            1.51148E-09  C4H6_2       1.29360E-18  C4H4_1       4.75003E-27
 C1H4O1       1.14083E-09  S4           1.12104E-18  C3H1         9.91558E-28
 O2S1         2.26895E-10  C4H8_5       6.89221E-19  C1H2O2_DIOXI 4.40433E-30
 C1H3         1.88514E-10  C4H8_1       5.18832E-19  C            1.00000E-30
 C1H4S1       1.76437E-10  C4H8_2       4.53214E-19  C2           1.00000E-30
 H2O1S1_HSOH  8.67082E-11  C4H8_3       3.93010E-19  C2H4O2_DIOXE 1.00000E-30
 C2H4O1_ACETA 2.61120E-11  C2H6O2       2.59417E-19  C2H4O3_123TR 1.00000E-30
 C2H2         1.43254E-11  C1H2         2.13894E-19  C2H4O3_124TR 1.00000E-30
 O1S1         1.05406E-11  C4H10_1      8.31953E-20  C3           1.00000E-30
 C1H1O1       9.19785E-12  C4H10_2      4.22679E-20  C4           1.00000E-30
 C1S1         5.40802E-12  C6H6         3.95182E-20  C4H1         1.00000E-30
```

```
 C2H4O2_ACETI 4.53120E-12  H2O2         2.47048E-20  C5           1.00000E-30
 H1O1         1.61961E-12  C4H6_4       1.91129E-20  C60          1.00000E-30
 O1S2         9.69426E-13  O3S1         1.73550E-20  O3           1.00000E-30
 C1H1O2       9.05180E-13  C4H6_1       1.14077E-20  S7           1.00000E-30
 S            7.19264E-13  O            6.56732E-21  S8           1.00000E-30
 S3           1.46179E-13  C4H6_3       6.48690E-21
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 t 500 2000 50
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex29 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   1000.000
...OK

 Phase Region from   1000.000     for:
     GAS
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
 Global test at  1.28000E+03 .... OK
 Global test at  1.38000E+03 .... OK
 Global test at  1.48000E+03 .... OK
 Global test at  1.58000E+03 .... OK
 Global test at  1.68000E+03 .... OK
 Global test at  1.78000E+03 .... OK
 Global test at  1.88000E+03 .... OK
 Global test at  1.98000E+03 .... OK
 Terminating at    2000.00
 Calculated   103 equilibria

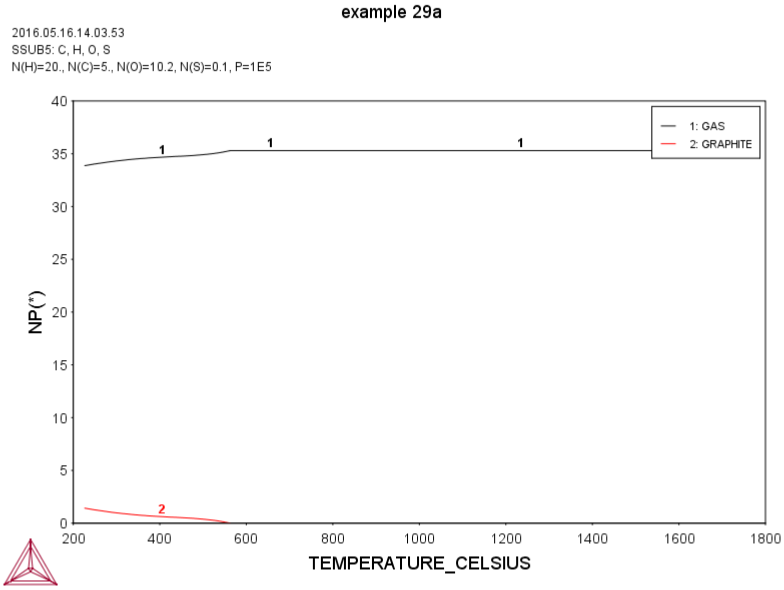
 Phase Region from   1000.000     for:
     GAS
 Global test at  9.20000E+02 .... OK
 Global check of adding phase at  8.35809E+02
 Calculated    19 equilibria

 Phase Region from    835.809     for:
     GAS
     GRAPHITE
 Global test at  7.60000E+02 .... OK
 Global test at  6.60000E+02 .... OK
 Global test at  5.60000E+02 .... OK
 Terminating at    500.000
 Calculated    37 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex29\tcex
 29.POLY3
POLY_3: post

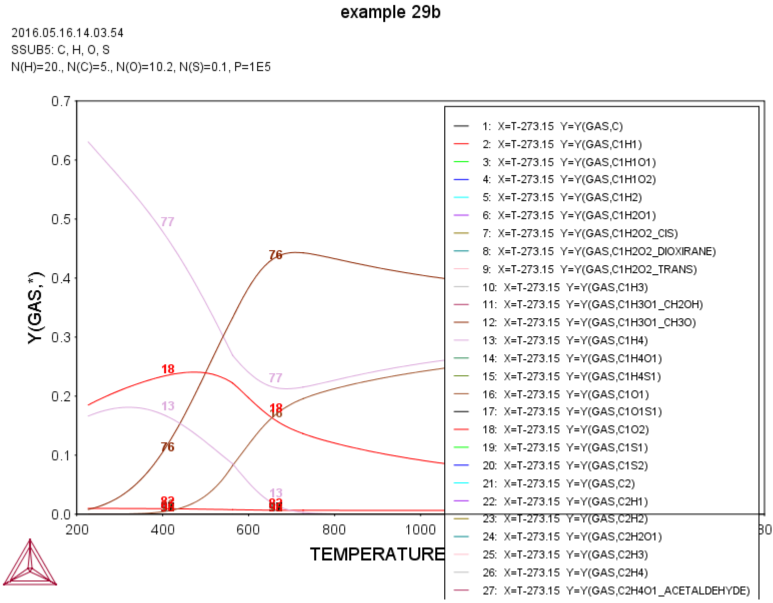
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

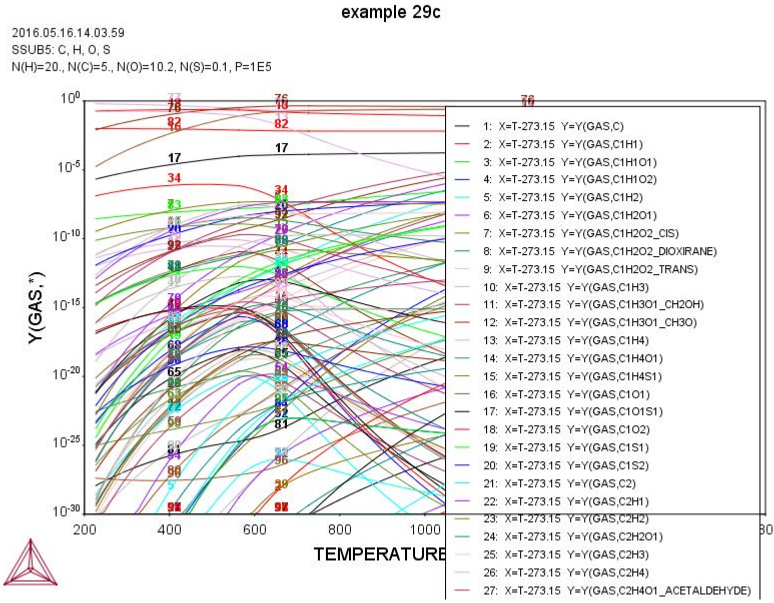
POST:
POST: @@ plot amount of phases, mainly gas!
POST: s-d-a x t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: s-l f
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 29a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



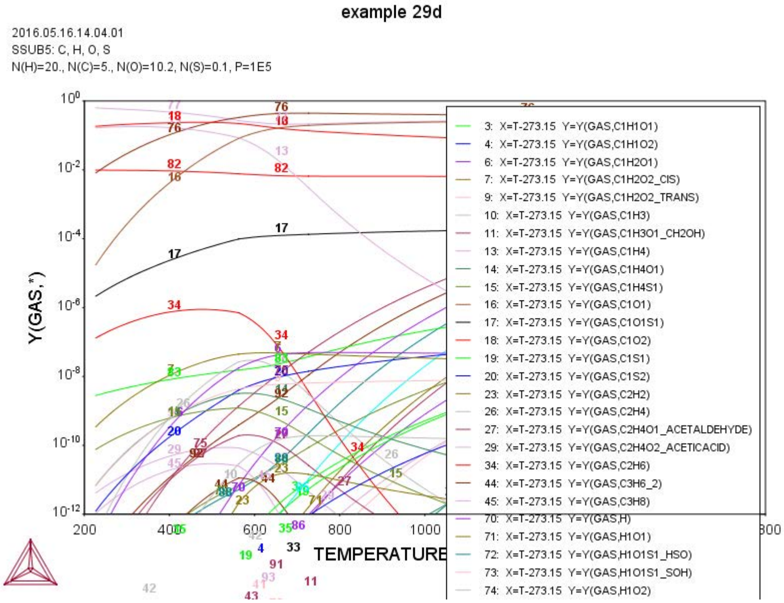
```
POST:
POST:Hit RETURN to continue
POST: @@ plot gas speciation. y(gas,*) are partial
POST: @@ pressures expressed in bar (as total pressure
POST: @@ is one bar!). Set labels on the lines.
POST: s-d-a y y(gas,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 29b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Set logarithmic axis
POST: s-ax-ty
   ... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : y
AXIS TYPE /LINEAR/: log
POST:
POST: set-title example 29c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Set scaling
POST: s-s y n 1e-12 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 29d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex30A

```
About Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex30A\tcex30A.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example of Scheil calculation for Al-4Mg-2Si-2Cu
SYS: @@    Part A: step-by-step calculation
SYS: @@
SYS:
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw user tcex30_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                       /-  DEFINED
TDB_USER: def-ele al cu mg si
 AL                       CU                       MG
 SI  DEFINED
TDB_USER: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 Reference REF1       missing close to line                    765
 Reference REF1       missing close to line                    767
 Reference REF1       missing close to line                    769
 Reference REF1       missing close to line                    771
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
 -OK-
TDB_USER: go p-3

 POLY version  3.32
POLY_3: s-c p=101325 n=1 t=1000 w(si)=0.02 w(mg)=0.04 w(cu)=0.02
POLY_3: c-e
 Using global minimization procedure
Calculated         24550 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 P=1.01325E5, N=1, T=1000, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.71965E+01
 Total Gibbs energy -4.56562E+04,  Enthalpy  3.06144E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      9.2731E-01  9.2000E-01 5.4982E-03 -4.3263E+04 SER
 CU                      8.5596E-03  2.0000E-02 5.9020E-07 -1.1925E+05 SER
 MG                      4.4759E-02  4.0000E-02 1.0064E-04 -7.6526E+04 SER
 SI                      1.9367E-02  2.0000E-02 1.1370E-03 -5.6367E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00  Mass fractions:
 AL  9.20000E-01  MG  4.00000E-02  CU  2.00000E-02  SI  2.00000E-02
POLY_3: @@ calculate liquidus temperature in order to choose
POLY_3: @@  a starting temperature where only liquid exists
POLY_3: c-st phase fcc_a1=fix 0
POLY_3: s-c t=none
POLY_3: c-e
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         24550 grid points in             0 s
    12 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 P=1.01325E5, N=1, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
 FIXED PHASES
 FCC_A1=0
 DEGREES OF FREEDOM 0

 Temperature    897.74 K (   624.59 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.71965E+01
 Total Gibbs energy -3.80281E+04,  Enthalpy  2.73862E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      9.2731E-01  9.2000E-01 8.2190E-03 -3.5838E+04 SER
 CU                      8.5596E-03  2.0000E-02 5.5836E-07 -1.0747E+05 SER
 MG                      4.4759E-02  4.0000E-02 1.2754E-04 -6.6933E+04 SER
 SI                      1.9367E-02  2.0000E-02 2.2867E-03 -4.5388E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00  Mass fractions:
 AL  9.20000E-01  MG  4.00000E-02  CU  2.00000E-02  SI  2.00000E-02

 FCC_A1                      Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
```

```
 AL  9.85194E-01  MG  1.12509E-02  CU  1.91685E-03  SI  1.63879E-03
POLY_3: show t
 T=897.74074
POLY_3:Hit RETURN to continue
POLY_3: s-c t
Value /897.7407448/: 900
POLY_3: c-st phase
Phase name(s): fcc_a1
Status: /ENTERED/: ENTERED
Start value, number of moles /0/: 0
POLY_3: c-e
 Using global minimization procedure
Calculated         24550 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 P=1.01325E5, N=1, T=900, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
 DEGREES OF FREEDOM 0

 Temperature    900.00 K (   626.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.71965E+01
 Total Gibbs energy -3.81928E+04,  Enthalpy  2.74567E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      9.2731E-01  9.2000E-01 8.1424E-03 -3.5998E+04 SER
 CU                      8.5596E-03  2.0000E-02 5.5930E-07 -1.0773E+05 SER
 MG                      4.4759E-02  4.0000E-02 1.2687E-04 -6.7141E+04 SER
 SI                      1.9367E-02  2.0000E-02 2.2488E-03 -4.5627E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00  Mass fractions:
 AL  9.20000E-01  MG  4.00000E-02  SI  2.00000E-02  CU  2.00000E-02
POLY_3: s-a-v 1 t
Min value /0/: 750 900 1
POLY_3:
POLY_3: ent var nl=1;
POLY_3: ent var nfcc=0;
POLY_3: ent var nl=np(liquid)*nl;
POLY_3: ent fun ns=1-nl;
POLY_3: ent var nfcc=nfcc+nl*np(fcc_a1);
POLY_3: ent var wsi=w(liquid,si);
POLY_3: ent var wmg=w(liquid,mg);
POLY_3: ent var wcu=w(liquid,cu);
POLY_3: ent tab tab1
Variable(s): t nl ns nfcc
&
POLY_3: s-c w(si)=wsi w(mg)=wmg w(cu)=wcu
POLY_3: save tcex30a y
POLY_3:
POLY_3: step
Option? /NORMAL/: eva
Variable name(s): wsi wmg wcu
 No initial equilibrium, using default
...OK

 Phase Region from    900.000     for:
     LIQUID
 Global check of adding phase at  8.97741E+02
 Calculated     5 equilibria

 Phase Region from    897.741     for:
     LIQUID
     FCC_A1
 Global test at  8.90000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  8.70000E+02 .... OK
 Global test at  8.60000E+02 .... OK
 Global check of adding phase at  8.57875E+02
 Calculated    43 equilibria

 Phase Region from    857.875     for:
     LIQUID
     FCC_A1
     MG2SI
 Global test at  8.50000E+02 .... OK
 Global test at  8.40000E+02 .... OK
 Global test at  8.30000E+02 .... OK
 Global test at  8.20000E+02 .... OK
 Global test at  8.10000E+02 .... OK
 Global test at  8.00000E+02 .... OK
 Global test at  7.90000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global check of adding phase at  7.78888E+02
 Calculated    82 equilibria

 Phase Region from    778.888     for:
     LIQUID
     ALCU_THETA
     FCC_A1
     MG2SI
 Global check of adding phase at  7.73208E+02
 Calculated     8 equilibria

 Phase Region from    773.208     for:
     LIQUID
     ALCU_THETA
     DIAMOND_A4
     FCC_A1
     MG2SI
 Calculated     2 equilibria

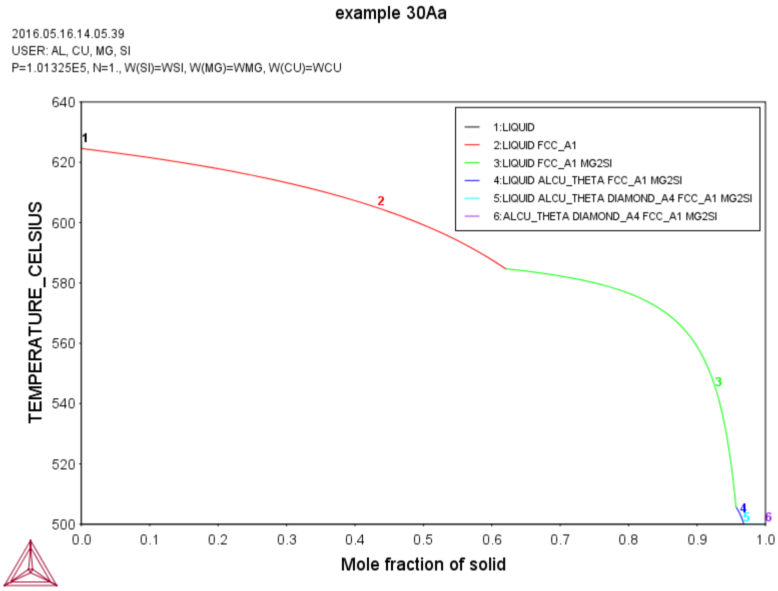
 Phase Region from    773.208     for:
     ALCU_THETA
     DIAMOND_A4
     FCC_A1
     MG2SI
 Global test at  7.66000E+02 .... OK
 Global test at  7.56000E+02 .... OK
 Terminating at    750.000
 Calculated    27 equilibria
```

```
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex30A\tce
 x30a.POLY3
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x tab1
COLUMN NUMBER /*/: 3
POST: s-d-a y t-c
POST:
POST: s-s-s y
AUTOMATIC SCALING  (Y OR N)  /N/: n
MIN VALUE : 500 640
POST: s-lab b
POST: se-ax-te x n
AXIS TEXT : Mole fraction of solid
POST: set-title example 30Aa
POST: plot
```

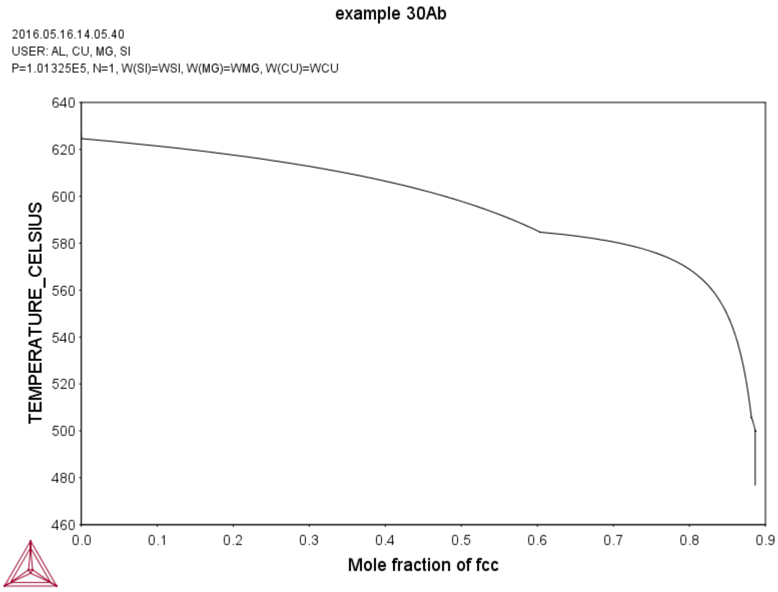


```
POST:
POST:Hit RETURN to continue
POST: back
POLY_3: read,,
POLY_3: po

  POLY-3 POSTPROCESSOR VERSION 3.2

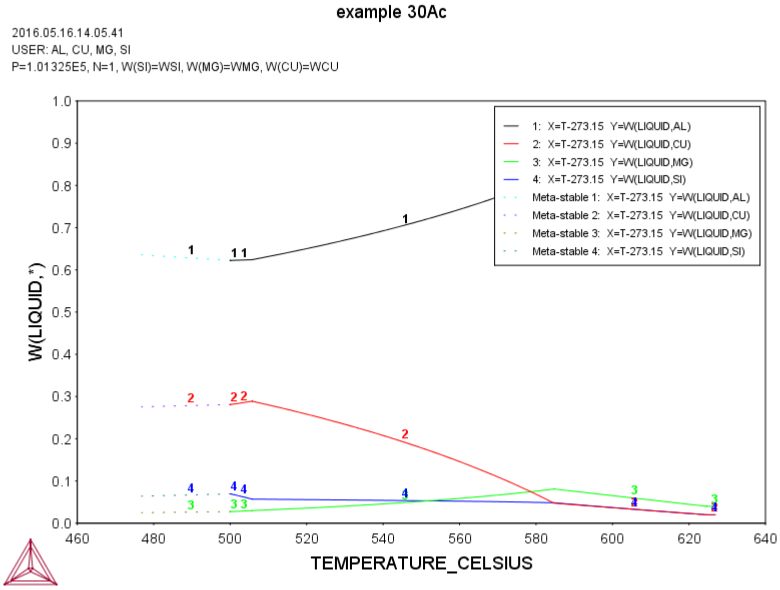

 Setting automatic diagram axes

POST: s-d-a x tab1
COLUMN NUMBER /*/: 4
POST: s-d-a y t-c
POST: se-ax-te x n
AXIS TEXT : Mole fraction of fcc
POST: set-title example 30Ab
POST:
POST: plot
```



```
POST:
POST:Hit RETURN to continue
POST: s-d-a x t-c
POST: s-d-a y w(liquid,*),,
POST: set-title example 30Ac
```

```
POST: s-l d
POST:
POST: plot
```



```
POST:
POST: set-inter
POST:
```

tcex30B

```
About Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex30B\tcex30B.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example of Scheil calculation for Al-4Mg-2Si-2Cu
SYS: @@    Part B: using SCHEIL module
SYS: @@
SYS: set-log ex30,,,
SYS:
SYS: go scheil
   ... the command in full is GOTO_MODULE
SCHEIL: start
   ... the command in full is START_WIZARD
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: user tcex30_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
Major element or alloy: al
Composition input in mass (weight) percent? /Y/:
1st alloying element: mg 4 si 2 cu 2
Next alloying element:
Temperature (C) /2000/: 800
 VA                      /-  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 AL  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MG  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CU  DEFINED


 This database has following phases for the defined system

 LIQUID:L                 AL12MG17                 ALCE_AMORPHOUS
 ALCUZN_T                 ALCU_DELTA               ALCU_EPSILON
 ALCU_ETA                 ALCU_PRIME               ALCU_THETA
 ALCU_ZETA                ALLI                     ALMG_BETA
 ALMG_EPS                 ALMG_GAMMA               ALMO
 ALM_D019                 ALND_AMORPHOUS           ALTI
 BCC_A2                   BCC_B2                   BCT_A5
 CBCC_A12                 CR3SI_A15                CRSI2
 CU19SI6_ETA              CU33SI7_DELTA            CU4SI_EPSILON
 CU56SI11_GAMMA           CU6Y                     CUB_A13
 CUB_A15                  CUMG2                    CUMGSI_SIGMA
 CUMGSI_TAU               CUZN_GAMMA               DIAMOND_A4
 FCC_A1                   GAMMA_D83                GAMMA_H
 HCP_A3                   HCP_ZN                   LAVES_C14
 LAVES_C15                LAVES_C36                MG24Y5
 MG2SI                    MG2Y                     MG2ZN11
 MG2ZN3                   MGY_GAMMA                MGZN
 PHI                      QPHASE                   SIV3
 SPHASE                   TAU                      VPHASE

Reject phase(s) /NONE/: *
 LIQUID:L                AL12MG17                ALCE_AMORPHOUS
 ALCUZN_T                ALCU_DELTA              ALCU_EPSILON
 ALCU_ETA                ALCU_PRIME              ALCU_THETA
 ALCU_ZETA               ALLI                    ALMG_BETA
 ALMG_EPS                ALMG_GAMMA              ALMO
 ALM_D019                ALND_AMORPHOUS          ALTI
 BCC_A2                  BCC_B2                  BCT_A5
 CBCC_A12                CR3SI_A15               CRSI2
 CU19SI6_ETA             CU33SI7_DELTA           CU4SI_EPSILON
 CU56SI11_GAMMA          CU6Y                    CUB_A13
 CUB_A15                 CUMG2                   CUMGSI_SIGMA
 CUMGSI_TAU              CUZN_GAMMA              DIAMOND_A4
 FCC_A1                  GAMMA_D83               GAMMA_H
 HCP_A3                  HCP_ZN                  LAVES_C14
 LAVES_C15               LAVES_C36               MG24Y5
 MG2SI                   MG2Y                    MG2ZN11
 MG2ZN3                  MGY_GAMMA               MGZN
 PHI                     QPHASE                  SIV3
 SPHASE                  TAU                     VPHASE
   REJECTED
Restore phase(s):: liquid fcc_a1 alcu_th mg2si diamond_a4 al12mg17
 LIQUID:L                FCC_A1                  ALCU_THETA
 MG2SI                   DIAMOND_A4              AL12MG17
   RESTORED
Restore phase(s): /NONE/:

 ........................................................

    The following phases are retained in this system:

 LIQUID:L                 AL12MG17                 ALCU_THETA
 DIAMOND_A4               FCC_A1                   MG2SI

 ........................................................

OK? /Y/: Y
 *** GAS INPUT IGNORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 Reference REF1       missing close to line                    765
 Reference REF1       missing close to line                    767
 Reference REF1       missing close to line                    769
```

```
 Reference REF1       missing close to line                    771
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
     1999/2003. '
 -OK-
Should any phase have a miscibility gap check? /N/: N
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/:
   ... the command in full is SET_NUMERICAL_LIMITS
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=1073.15, W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0
To form FCC_A1#1 the condition is set to T=897.740744839
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
   ... the command in full is ADVANCED_OPTIONS
   ... the command in full is STEP_WITH_OPTIONS
...OK

 Phase Region from    897.731     for:
     LIQUID
     FCC_A1
 Global check of removing phase at  8.97741E+02
 Calculated     3 equilibria

 Phase Region from    897.741     for:
     LIQUID
 Terminating at    897.831
 Calculated     4 equilibria

 Phase Region from    897.731     for:
     LIQUID
     FCC_A1
 Global test at  8.89731E+02 .... OK
 Global test at  8.79731E+02 .... OK
 Global test at  8.69731E+02 .... OK
 Global test at  8.59731E+02 .... OK
 Global check of adding phase at  8.57535E+02
 Calculated    43 equilibria

 Phase Region from    857.535     for:
     LIQUID
     FCC_A1
     MG2SI
 Global test at  8.49731E+02 .... OK
 Global test at  8.39731E+02 .... OK
 Global test at  8.29731E+02 .... OK
 Global check of removing phase at  8.26196E+02
 Calculated    34 equilibria

 Phase Region from    826.196     for:
     FCC_A1
     MG2SI
 Calculated     4 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex30B\SCH
 EIL_676.POLY3

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes


  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

   ... the command in full is ENTER_SYMBOL
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 An EXP file c:\jenkins\WORKSP~1\THERMO~1\examples\tcex30B\SCHEIL_EQ_676.EXP
 has been created to store the equilibrium solidification results.
   ... the command in full is READ_WORKSPACES
  CALCULATING SCHEIL SOLDIFICATION
   ... the command in full is SET_NUMERICAL_LIMITS

     T(C)      fraction solid

   624.6807       0.000000

  PHASE REGION:LIQUID + FCC_A1

     T(C)      fraction solid

   624.5870      0.1358787E-03
   623.5870      0.3532418E-01
   622.5870      0.6836458E-01
   621.5870      0.9944066E-01
   620.5870      0.1287161
   619.5870      0.1563371
   618.5870      0.1824349
   617.5870      0.2071274
   616.5870      0.2305208
   615.5870      0.2527111
   614.5870      0.2737852
   613.5870      0.2938222
   612.5870      0.3128937
   611.5870      0.3310652
   610.5870      0.3483963
   609.5870      0.3649419
   608.5870      0.3807520
   607.5870      0.3958726
   606.5870      0.4103460
   605.5870      0.4242113
   604.5870      0.4375043
   603.5870      0.4502583
   602.5870      0.4625042
   601.5870      0.4742703
   600.5870      0.4855831
```

```
 599.5870      0.4964672
 598.5870      0.5069455
 597.5870      0.5170392
 596.5870      0.5267681
 595.5870      0.5361509
 594.5870      0.5452047
 593.5870      0.5539459
 592.5870      0.5623895
 591.5870      0.5705498
 590.5870      0.5784402
 589.5870      0.5860731
 588.5870      0.5934603
 587.5870      0.6006129
 586.5870      0.6075414
 585.5870      0.6142556
 584.7432      0.6197601

PHASE REGION:LIQUID + FCC_A1 + MG2SI

   T(C)      fraction solid

 584.7120      0.6204291
 583.7120      0.6580982
 582.7120      0.6889903
 581.7120      0.7147690
 580.7120      0.7365965
 579.7120      0.7553093
 578.7120      0.7715239
 577.7120      0.7857051
 576.7120      0.7982095
 575.7120      0.8093153
 574.7120      0.8192426
 573.7120      0.8281678
 572.7120      0.8362341
 571.7120      0.8435586
 570.7120      0.8502382
 569.7120      0.8563537
 568.7120      0.8619730
 567.7120      0.8671536
 566.7120      0.8719445
 565.7120      0.8763876
 564.7120      0.8805191
 563.7120      0.8843705
 562.7120      0.8879691
 561.7120      0.8913386
 560.7120      0.8945002
 559.7120      0.8974722
 558.7120      0.9002713
 557.7120      0.9029118
 556.7120      0.9054068
 555.7120      0.9077679
 554.7120      0.9100055
 553.7120      0.9121290
 552.7120      0.9141468
 551.7120      0.9160667
 550.7120      0.9178954
 549.7120      0.9196393
 548.7120      0.9213042
 547.7120      0.9228952
 546.7120      0.9244172
 545.7120      0.9258745
 544.7120      0.9272712
 543.7120      0.9286109
 542.7120      0.9298971
 541.7120      0.9311328
 540.7120      0.9323211
 539.7120      0.9334645
 538.7120      0.9345656
 537.7120      0.9356266
 536.7120      0.9366498
 535.7120      0.9376371
 534.7120      0.9385904
 533.7120      0.9395114
 532.7120      0.9404018
 531.7120      0.9412630
 530.7120      0.9420964
 529.7120      0.9429035
 528.7120      0.9436854
 527.7120      0.9444432
 526.7120      0.9451783
 525.7120      0.9458914
 524.7120      0.9465837
 523.7120      0.9472560
 522.7120      0.9479092
 521.7120      0.9485441
 520.7120      0.9491615
 519.7120      0.9497621
 518.7120      0.9503466
 517.7120      0.9509157
 516.7120      0.9514700
 515.7120      0.9520100
 514.7120      0.9525364
 513.7120      0.9530496
 512.7120      0.9535502
 511.7120      0.9540386
 510.7120      0.9545153
 509.7120      0.9549808
 508.7120      0.9554354
 507.7120      0.9558795
 506.7120      0.9563136
 505.7432      0.9567248

PHASE REGION:LIQUID + ALCU_THETA + FCC_A1 + MG2SI

   T(C)      fraction solid

 505.7120      0.9568034
 504.7120      0.9595410
 503.7120      0.9618872
 502.7120      0.9639256
 501.7120      0.9657170
 500.7120      0.9673065

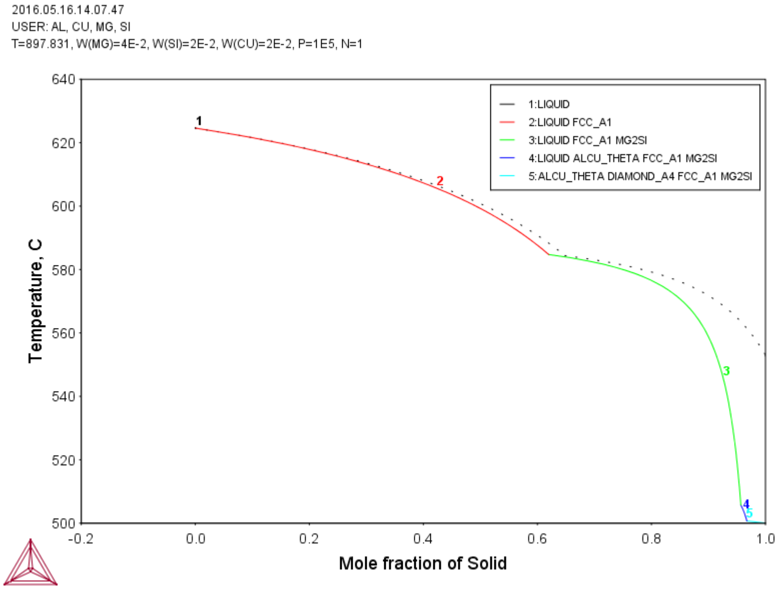
PHASE REGION:ALCU_THETA + DIAMOND_A4 + FCC_A1 + MG2SI

   T(C)      fraction solid
```

```
   500.0557      1.0000000

 Hint: move the last function to the first equilibrium where it is used

   ... the command in full is SET_LABEL_CURVE_OPTION
   ... the command in full is APPEND_EXPERIMENTAL_DATA
```



```
   ... the command in full is APPEND_EXPERIMENTAL_DATA

  ...........................................................

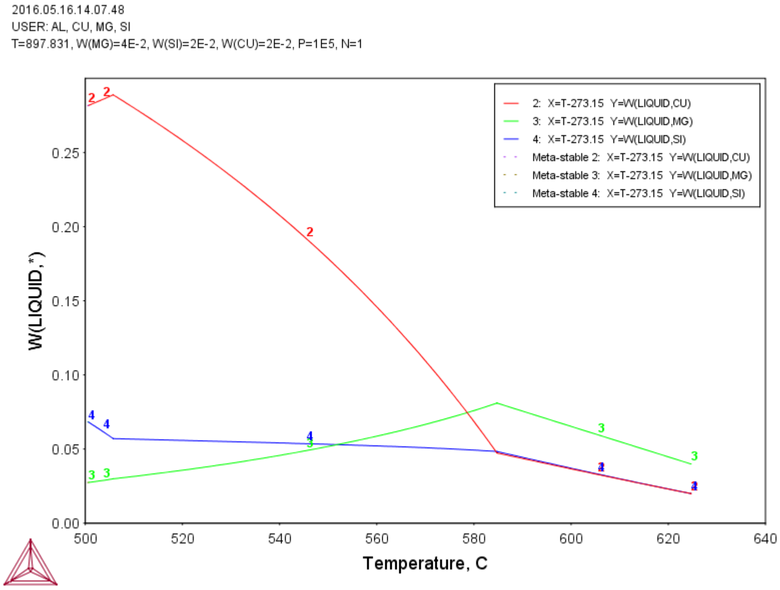
        The following axis variables are available

             T --- Temperature in Celsius
         NL/BL --- Mole/mass fraction of liquid
         NS/BS --- Mole/mass fraction of all solid phases
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
      W(ph,el) --- Weight fraction of an element in a phase
      X(ph,el) --- Mole fraction of an element in a phase
      Y(ph,el) --- Site fraction of an element in a phase
     NN(ph,el) --- Distribution of an element in a phases
         NH/BH --- Heat release and Latent heat per mole/gram
        CP/BCP --- Apparent heat capacity per mole/gram
     NV/NV(ph) --- Molar volume of the system or a phase
     DS/DS(ph) --- Average density of the system or a phase
            BT --- Apparent volumetric TEC of the system

  "el" and "ph" are name of element and phase, respectively
     "*" can be used as a wild character for "el" and "ph"

  ..........................................................

POST:
POST:Hit RETURN to continue
POST: s-d-a x t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(liquid,*),,,,,,
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s y n 0 0.3
   ... the command in full is SET_SCALING_STATUS
POST: set-lab F
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot,,,,
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex31

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex31.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculations of CVM and comparisons with sublattices
SYS: @@ of a fictitious A B system.
SYS: @@ Also shows how to overlay diagrams from two calculations
SYS: @@
SYS:
SYS: set-log ex31,,,
SYS:
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES:
GES: @@ Enter the elements and their reference states
GES: e-e A B
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
GES: a-e-d A
   ... the command in full is AMEND_ELEMENT_DATA
NEW STABLE ELEMENT REFERENCE /UNKNOWN/: FCC
NEW ATOMIC MASS /0/: 10
NEW H(298.15)-H(0) /0/: 0
NEW S(298.15) /0/: 0
Default element reference state symbol index /1/: 1
GES: a-e-d B
   ... the command in full is AMEND_ELEMENT_DATA
NEW STABLE ELEMENT REFERENCE /BETA_RHOMBO_B/: FCC
NEW ATOMIC MASS /10.811/: 10
NEW H(298.15)-H(0) /1222/: 0
NEW S(298.15) /5.9/: 0
Default element reference state symbol index /1/: 1
GES:
GES: @@ =====================================================
GES: @@ These species represent the clusters. 4 clusters A3B are needed
GES: @@ as the B atom can be on 4 different sublattices etc.
GES: e-sp S0 A
   ... the command in full is ENTER_SPECIES
GES: e-sp S11 A.75B.25
   ... the command in full is ENTER_SPECIES
GES: e-sp S12 A.75B.25
   ... the command in full is ENTER_SPECIES
GES: e-sp S13 A.75B.25
   ... the command in full is ENTER_SPECIES
GES: e-sp S14 A.75B.25
   ... the command in full is ENTER_SPECIES
GES: e-sp S21 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S22 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S23 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S24 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S25 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S26 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S31 A.25B.75
   ... the command in full is ENTER_SPECIES
GES: e-sp S32 A.25B.75
   ... the command in full is ENTER_SPECIES
GES: e-sp S33 A.25B.75
   ... the command in full is ENTER_SPECIES
GES: e-sp S34 A.25B.75
   ... the command in full is ENTER_SPECIES
GES: e-sp S4 B
   ... the command in full is ENTER_SPECIES
GES:
GES: @@ ================================================================
GES: @@ This function describes the bond energy A-B at equiatomic composition
GES: e-sy fun UIJ
   ... the command in full is ENTER_SYMBOL
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: -100*R;
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: N
GES:
GES: @@ These functions describe the end-member energies at A3B, A2B2 and AB3
GES: @@ respectivly.  In the simplest case, like here, they are just the
GES: @@ bond energy multiplied with 3, 4 and 3 respectively.
GES: e-sy fun GA3B1,,3*UIJ;,,,
   ... the command in full is ENTER_SYMBOL
GES: e-sy fun GA2B2,,4*UIJ;,,,
   ... the command in full is ENTER_SYMBOL
GES: e-sy fun GA1B3,,3*UIJ;,,,
   ... the command in full is ENTER_SYMBOL
GES:
GES: @@ ==================================================
GES: @@ This is the fcc phase with CVM for both lro and sro
GES: e-ph CVM_TET
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S4
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES: E-PAR G(C,S11),,GA3B1;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(C,S12),,GA3B1;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
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GES: E-PAR G(C,S13),,GA3B1;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(C,S14),,GA3B1;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(C,S21),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S22),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S23),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S24),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S25),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S26),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S31),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(C,S32),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(C,S33),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(C,S34),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: l-d,,,,
   ... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT       DATE 2016- 5-16
 FROM DATABASE: User data 2016.05.16

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  1 A    FCC                       1.0000E+01  0.0000E+00  0.0000E+00
  2 B    FCC                       1.0000E+01  0.0000E+00  0.0000E+00


 SPECIES                                    STOICHIOMETRY
   1 A                                      A
   2 B                                      B
   3 S0                                     A
   4 S11                                    A0.75B0.25
   5 S12                                    A0.75B0.25
   6 S13                                    A0.75B0.25
   7 S14                                    A0.75B0.25
   8 S21                                    A0.5B0.5
   9 S22                                    A0.5B0.5
  10 S23                                    A0.5B0.5
  11 S24                                    A0.5B0.5
  12 S25                                    A0.5B0.5
  13 S26                                    A0.5B0.5
  14 S31                                    A0.25B0.75
  15 S32                                    A0.25B0.75
  16 S33                                    A0.25B0.75
  17 S34                                    A0.25B0.75
  18 S4                                     B



 CVM_TET
    CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
    S4

      G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
      G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)  = +GA3B1
      G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)  = +GA3B1
      G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)  = +GA3B1
      G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)  = +GA3B1
      G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)  = +GA1B3
      G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)  = +GA1B3
      G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)  = +GA1B3
      G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)  = +GA1B3
      G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 103 UIJ       20000000 -100*R
 104 GA3B1     20000000 +3*UIJ
 105 GA2B2     20000000 +4*UIJ
 106 GA1B3     20000000 +3*UIJ


GES:
GES:Hit RETURN to continue
GES: @@ ========================================
GES: @@ This is an fcc phase with no sro but lro
GES: @@ described with the sublattice model
GES: E-PH LRO
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 4
NUMBER OF SITES IN SUBLATTICE  1 /1/: .25
NUMBER OF SITES IN SUBLATTICE  2 /1/: .25
NUMBER OF SITES IN SUBLATTICE  3 /1/: .25
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NUMBER OF SITES IN SUBLATTICE  4 /1/: .25
 CONSTITUENTS IN SUBLATTICE                      1
NAME OF CONSTITUENT: A B;
 CONSTITUENTS IN SUBLATTICE                      2
NAME OF CONSTITUENT: A B;
 CONSTITUENTS IN SUBLATTICE                      3
NAME OF CONSTITUENT: A B;
 CONSTITUENTS IN SUBLATTICE                      4
NAME OF CONSTITUENT: A B;
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES:
GES: E-PAR G(L,A:A:A:B),,GA3B1;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(L,A:A:B:A),,GA3B1;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(L,A:B:A:A),,GA3B1;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:B:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(L,B:A:A:A),,GA3B1;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(L,A:B:B:B),,GA1B3;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:B:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(L,B:A:B:B),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(L,B:B:A:B),,GA1B3;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:B:A:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(L,B:B:B:A),,GA1B3;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:B:B:A;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(L,A:A:B:B),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,A:B:A:B),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,B:A:A:B),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:A:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,A:B:B:A),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:B:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,B:A:B:A),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,B:B:A:A),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: l-p-d lro
   ... the command in full is LIST_PHASE_DATA


 LRO
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: A,B : A,B : A,B : A,B

      G(LRO,A:A:A:A;0)-G(FCC,A;0) = 0.0
      G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)  = +GA3B1
      G(LRO,A:B:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)  = +GA3B1
      G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)  = +GA3B1
      G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(LRO,A:B:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(LRO,B:B:B:A;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)  = +GA1B3
      G(LRO,A:A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)  = +GA3B1
      G(LRO,B:A:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(LRO,A:B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(LRO,B:B:A:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)  = +GA1B3
      G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)  = +GA2B2
      G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)  = +GA1B3
      G(LRO,A:B:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)  = +GA1B3
      G(LRO,B:B:B:B;0)-G(FCC,B;0) = 0.0
GES:
GES: @@ ============================================================
GES: @@ This is the fcc phase with no sro and no lro.  The regular
GES: @@ parameters is simply 12 times the bond energy as the ;1 and ;2
GES: @@ parameters cancel when GA1B3=GA3B1=0.75*GA2B2
GES: e-ph fcc_a1
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES:
GES: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;0)
GES: e-par l(fcc,a,b;1),,2*GA3B1-2*GA1B3;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;1)
GES: e-par l(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3;,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;2)
GES: l-p-d fcc
   ... the command in full is LIST_PHASE_DATA


 FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
      G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
      L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
      L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3
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      L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3
GES:
GES: @@ Finally we add together the LRO phase with the disordered FCC
GES: @@ Note that the parameters in LRO will give zero contribution
GES: @@ when the phase is disordered
GES: amend-phase LRO dis FCC
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: @@
GES: @@ This is the secret way to set CVM entropy calculation
GES: am-ph cvm stat 02204030
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: l-p-d cvm
   ... the command in full is LIST_PHASE_DATA


 CVM_TET
 $ CVM-SRO ENTROPY CONTRIBUTION
    CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
    S4

      G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
      G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0
GES:
GES:Hit RETURN to continue
GES: @@ We need 3 CVM phases for the L10, L12 and disordered states
GES: am-ph cvm
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER /2/: 3
 GIVE FOR COMPOSITION SET                       2
Major constituent(s) for sublattice 1: /$/: s11
 GIVE FOR COMPOSITION SET                       3
Major constituent(s) for sublattice 1: /$/: none
GES:
GES: am-ph cvm maj
   ... the command in full is AMEND_PHASE_DESCRIPTION
Composition set /1/: 1
Major constituent(s) for sublattice 1: /S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S/: S25
GES:
GES: @@ Also for the sublattice phase we need 3 composition sets
GES: am-ph lro
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER /2/: 3
 GIVE FOR COMPOSITION SET                       2
Major constituent(s) for sublattice 1: /A B/: *
Major constituent(s) for sublattice 2: /A B/: *
Major constituent(s) for sublattice 3: /A B/: *
Major constituent(s) for sublattice 4: /A B/: *
 GIVE FOR COMPOSITION SET                       3
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: B
Major constituent(s) for sublattice 4: /A B/: B
GES: am-ph lro
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: maj
Composition set /1/: 1
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: A
Major constituent(s) for sublattice 4: /A B/: B
GES:
GES: l-d,,,,
   ... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE: User data 2016.05.16

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  1 A    FCC                       1.0000E+01  0.0000E+00  0.0000E+00
  2 B    FCC                       1.0000E+01  0.0000E+00  0.0000E+00


 SPECIES                                      STOICHIOMETRY
   1 A                                        A
   2 B                                        B
   3 S0                                       A
   4 S11                                      A0.75B0.25
   5 S12                                      A0.75B0.25
   6 S13                                      A0.75B0.25
   7 S14                                      A0.75B0.25
   8 S21                                      A0.5B0.5
   9 S22                                      A0.5B0.5
  10 S23                                      A0.5B0.5
  11 S24                                      A0.5B0.5
  12 S25                                      A0.5B0.5
  13 S26                                      A0.5B0.5
  14 S31                                      A0.25B0.75
  15 S32                                      A0.25B0.75
  16 S33                                      A0.25B0.75
  17 S34                                      A0.25B0.75
  18 S4                                       B
```

```
 CVM_TET
 $ CVM-SRO ENTROPY CONTRIBUTION
    CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
    S4

      G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
      G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0


 FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF LRO
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
      G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
      L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
      L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3
      L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3


 LRO
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: A,B : A,B : A,B : A,B

      G(LRO,A:A:A:A;0) = 0.0
      G(LRO,B:A:A:A;0) = +GA3B1
      G(LRO,A:B:A:A;0) = +GA3B1
      G(LRO,B:B:A:A;0) = +GA2B2
      G(LRO,A:A:B:A;0) = +GA3B1
      G(LRO,B:A:B:A;0) = +GA2B2
      G(LRO,A:B:B:A;0) = +GA2B2
      G(LRO,B:B:B:A;0) = +GA1B3
      G(LRO,A:A:A:B;0) = +GA3B1
      G(LRO,B:A:A:B;0) = +GA2B2
      G(LRO,A:B:A:B;0) = +GA2B2
      G(LRO,B:B:A:B;0) = +GA1B3
      G(LRO,A:A:B:B;0) = +GA2B2
      G(LRO,B:A:B:B;0) = +GA1B3
      G(LRO,A:B:B:B;0) = +GA1B3
      G(LRO,B:B:B:B;0) = 0.0

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 103 UIJ       20000000 -100*R
 104 GA3B1     20000000 +3*UIJ
 105 GA2B2     20000000 +4*UIJ
 106 GA1B3     20000000 +3*UIJ


GES:Hit RETURN to continue
GES: @@ ==========================================
GES: @@ Now we can start calculating
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3:
POLY_3: @@ turn global minimization off
POLY_3: set-min-op
   ... the command in full is SET_MINIMIZATION_OPTIONS
 This command is DEPRECATED and to be removed in the future!
 Settings for global minimization:
 Use global minimization /Y/: n
 Settings for general calculations:
 Force positive definite Phase Hessian /Y/: n
 Control minimization step size /Y/:
POLY_3:
POLY_3: L-C
   ... the command in full is LIST_CONDITIONS
 DEGREES OF FREEDOM 4
POLY_3: S-C T=60 P=1E5 N=1 X(B)=.4
   ... the command in full is SET_CONDITION
POLY_3: @@
POLY_3: @@ First calculate just with the full CVM phases
POLY_3: ch-st ph *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: ch-st ph cvm cvm#2 cvm#3=ent 1
   ... the command in full is CHANGE_STATUS
POLY_3: @@
POLY_3: @@ L10 ordering, setting start composition essential ....
POLY_3: @@ The initial fraction of each species is bascially calculated as the
POLY_3: @@ product of the site fraction on each sublattice.
POLY_3: s-s-c cvm
   ... the command in full is SET_START_CONSTITUTION
Y(CVM_TET,S0) /1/: .002
Y(CVM_TET,S11) /1/: 1.16e-3
Y(CVM_TET,S12) /1/: 1.76e-1
Y(CVM_TET,S13) /1/: 1.16e-3
Y(CVM_TET,S14) /1/: 1.76e-1
Y(CVM_TET,S21) /1/: 7.56e-3
Y(CVM_TET,S22) /1/: 5e-5
Y(CVM_TET,S23) /1/: 7.56e-3
Y(CVM_TET,S24) /1/: 7.56e-3
```

```
Y(CVM_TET,S25) /1/: 6.08e-1
Y(CVM_TET,S26) /1/: 7.56e-3
Y(CVM_TET,S31) /1/: 1.76e-3
Y(CVM_TET,S32) /1/: 2e-5
Y(CVM_TET,S33) /1/: 1.76e-3
Y(CVM_TET,S34) /1/: 2e-5
Y(CVM_TET,S4) /1/: 4e-7
POLY_3:
POLY_3: @@ L12 ordering
POLY_3: s-s-c cvm#2
   ... the command in full is SET_START_CONSTITUTION
Y(CVM_TET#2,S0) /1/: .002
Y(CVM_TET#2,S11) /1/: .46
Y(CVM_TET#2,S12) /1/: .0078
Y(CVM_TET#2,S13) /1/: .0078
Y(CVM_TET#2,S14) /1/: .0078
Y(CVM_TET#2,S21) /1/: .168
Y(CVM_TET#2,S22) /1/: .168
Y(CVM_TET#2,S23) /1/: .168
Y(CVM_TET#2,S24) /1/: .0012
Y(CVM_TET#2,S25) /1/: .0012
Y(CVM_TET#2,S26) /1/: .0012
Y(CVM_TET#2,S31) /1/: 5e-6
Y(CVM_TET#2,S32) /1/: .002
Y(CVM_TET#2,S33) /1/: .002
Y(CVM_TET#2,S34) /1/: .002
Y(CVM_TET#2,S4) /1/: 1e-6
POLY_3:
POLY_3: s-s-c cvm#3 *
   ... the command in full is SET_START_CONSTITUTION
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    19 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xnp
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=60, P=1E5, N=1, X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     60.00 K (  -213.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.10213E+03,  Enthalpy -2.96850E+03,  Volume  0.00000E+00

 Component               Moles      M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 2.0465E-02 -1.9401E+03 SER
 B                       4.0000E-01  4.0000E-01 6.0538E-05 -4.8452E+03 SER

 CVM_TET                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.6950E-01, Mass 5.6950E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  5.89207E-01  B  4.10793E-01
 Constitution:
 S25  5.78440E-01  S23  1.28068E-02  S33  4.13398E-03  S22  2.56479E-04
 S14  1.76120E-01  S21  1.28068E-02  S0   3.76373E-03  S32  1.15932E-04
 S12  1.76120E-01  S24  1.28068E-02  S13  2.78465E-03  S34  1.15932E-04
 S26  1.28068E-02  S31  4.13398E-03  S11  2.78465E-03  S4   3.67798E-06

 CVM_TET#2                   Status ENTERED     Driving force  0.0000E+00
 Moles 4.3050E-01, Mass 4.3050E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.14278E-01  B  3.85722E-01
 Constitution:
 S11  4.21306E-01  S14  1.38900E-02  S33  4.69234E-03  S25  3.19866E-03
 S23  1.69717E-01  S13  1.38900E-02  S34  4.69234E-03  S24  3.19866E-03
 S21  1.69717E-01  S12  1.38900E-02  S0   4.13973E-03  S31  5.05554E-05
 S22  1.69717E-01  S32  4.69234E-03  S26  3.19866E-03  S4   8.90403E-06

 CVM_TET#3                   Status ENTERED     Driving force -1.0709E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.09450E-01  B  3.90550E-01
 Constitution:
 S14  1.09230E-01  S23  8.47466E-02  S21  8.47466E-02  S33  8.87560E-03
 S13  1.09230E-01  S26  8.47466E-02  S22  8.47466E-02  S34  8.87560E-03
 S12  1.09230E-01  S25  8.47466E-02  S0   1.86436E-02  S31  8.87560E-03
 S11  1.09230E-01  S24  8.47466E-02  S32  8.87560E-03  S4   4.53364E-04
POLY_3:Hit RETURN to continue
POLY_3: s-c t=40
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    18 ITS,  CPU TIME USED   0 SECONDS
POLY_3: s-s-c cvm#3 *
   ... the command in full is SET_START_CONSTITUTION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    18 ITS,  CPU TIME USED   0 SECONDS
POLY_3: L-E
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNP/:
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=40, P=1E5, N=1, X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     40.00 K (  -233.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.06232E+03,  Enthalpy -2.98938E+03,  Volume  0.00000E+00

 Component               Moles      M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 4.1519E-03 -1.8239E+03 SER
 B                       4.0000E-01  4.0000E-01 3.7621E-07 -4.9199E+03 SER

 CVM_TET                     Status ENTERED     Driving force  0.0000E+00
 Moles 6.6953E-01, Mass 6.6953E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  5.88358E-01  B  4.11642E-01
 Constitution:
 S25  6.26368E-01  S24  4.57470E-03  S33  6.44301E-04  S22  1.02379E-05
```

```
 S14  1.76201E-01  S23  4.57470E-03  S31  6.44301E-04  S34  4.02672E-06
 S12  1.76201E-01  S21  4.57470E-03  S13  4.60814E-04  S32  4.02672E-06
 S26  4.57470E-03  S0   7.03194E-04  S11  4.60814E-04  S4   2.24689E-08

 CVM_TET#2                   Status ENTERED     Driving force  0.0000E+00
 Moles 3.3047E-01, Mass 3.3047E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.23586E-01  B  3.76414E-01
 Constitution:
 S11  4.81572E-01  S14  4.56422E-03  S32  7.57611E-04  S26  4.03145E-04
 S21  1.66859E-01  S12  4.56422E-03  S34  7.57611E-04  S24  4.03145E-04
 S23  1.66859E-01  S13  4.56422E-03  S0   6.77145E-04  S31  4.66624E-07
 S22  1.66859E-01  S33  7.57611E-04  S25  4.03145E-04  S4   4.50770E-08

 CVM_TET#3                   Status ENTERED     Driving force -3.4466E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.15550E-01  B  3.84450E-01
 Constitution:
 S11  1.12327E-01  S21  8.23389E-02  S25  8.23389E-02  S33  8.17828E-03
 S13  1.12327E-01  S22  8.23389E-02  S24  8.23389E-02  S34  8.17828E-03
 S14  1.12327E-01  S23  8.23389E-02  S0   2.33728E-02  S31  8.17828E-03
 S12  1.12327E-01  S26  8.23389E-02  S32  8.17828E-03  S4   5.71422E-04
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 x(b) 0 .5,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 0 100,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex31a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map -
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.116E-01  4.000E+01
     CVM_TET
  ** CVM_TET#2
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
 31a.POLY3
 Terminating at diagram limit
 CALCULATED    27 EQUILIBRIA

 Phase region boundary   2 at:   4.116E-01  4.000E+01
     CVM_TET
  ** CVM_TET#2
 CALCULATED    26 EQUILIBRIA

 Phase region boundary   2 at:   4.240E-01  8.061E+01
     CVM_TET
  ** CVM_TET#2
     CVM_TET#3

 Phase region boundary   2 at:   4.147E-01  8.061E+01
  ** CVM_TET#2
     CVM_TET#3
 *** SORRY CANNOT CONTINUE ***    4

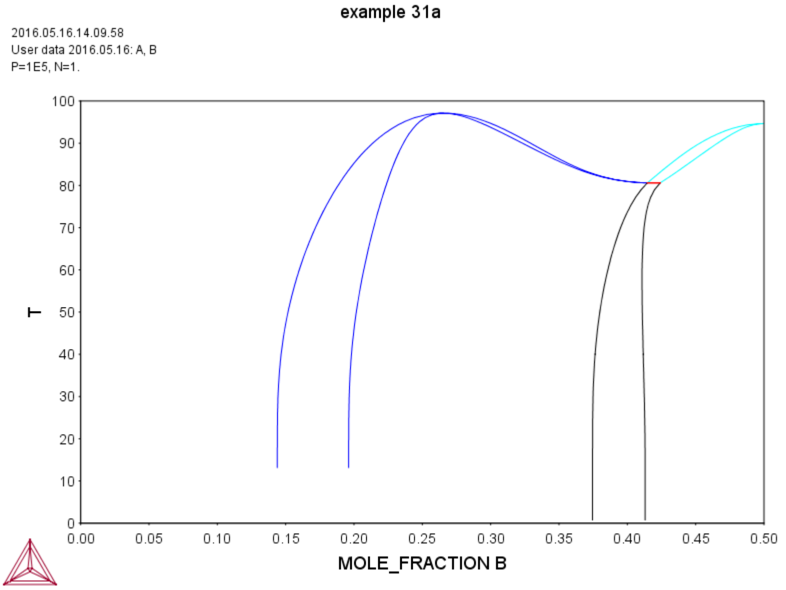
 CALCULATED    95 EQUILIBRIA

 Phase region boundary   2 at:   4.240E-01  8.061E+01
     CVM_TET
  ** CVM_TET#3
 Terminating at diagram limit
 CALCULATED    24 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
 31a.POLY3
 CPU time for mapping                      0  seconds
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x m-f b
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 0.5
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 100
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 31a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Make an experimental data file to overlay the next calculation
POST: make tcex31 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY_3: @@
POLY_3: @@ It is interesting to compare with a CEF without any sro contribution.
POLY_3: @@ This is the classical FCC ordering diagram first calculated
POLY_3: @@ manually by W Shockley, J chem Phys, 6, (1938) p 130
POLY_3: read tcex31a
   ... the command in full is READ_WORKSPACES
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p lro lro#2 lro#3=ent 0
   ... the command in full is CHANGE_STATUS
POLY_3: s-c t=70 x(b)=.4
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    32 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=70, P=1E5, N=1., X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     70.00 K (  -203.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.08055E+03,  Enthalpy -2.95310E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 4.7333E-02 -1.7755E+03 SER
 B                       4.0000E-01  4.0000E-01 1.7400E-04 -5.0382E+03 SER

 LRO                      ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 2.6762E-01, Mass 2.6762E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.74559E-01  B  3.25441E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99692E-01  A  3.08116E-04

 LRO#2                    DISORD Status ENTERED   Driving force -4.6485E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.45965E-01  B  3.54035E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01

 LRO#3                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 7.3238E-01, Mass 7.3238E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  5.72756E-01  B  4.27244E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.99661E-01  B  3.38612E-04
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.99661E-01  B  3.38612E-04
 Sublattice  3,  Number of sites  2.5000E-01
 B  8.54150E-01  A  1.45850E-01
 Sublattice  4,  Number of sites  2.5000E-01
```

```
 B  8.54150E-01  A  1.45850E-01
POLY_3:Hit RETURN to continue
POLY_3: s-s-c lro#3
   ... the command in full is SET_START_CONSTITUTION
Y(LRO#3,A) /.9996613878/:
Y(LRO#3,B) /3.386121641E-04/:
Y(LRO#3,A#2) /.9996613878/:
Y(LRO#3,B#2) /3.386121641E-04/:
Y(LRO#3,A#3) /.1458499446/: 0.0001
Y(LRO#3,B#3) /.8541500554/: 0.9999
Y(LRO#3,A#4) /.1458499446/: .6
Y(LRO#3,B#4) /.8541500554/: .4
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    23 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=70, P=1E5, N=1., X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     70.00 K (  -203.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.09267E+03,  Enthalpy -2.98506E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 4.1721E-02 -1.8489E+03 SER
 B                       4.0000E-01  4.0000E-01 1.9961E-04 -4.9583E+03 SER

 LRO                      ORD    Status ENTERED   Driving force -3.9691E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.68667E-01  B  3.31333E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99690E-01  A  3.09926E-04

 LRO#2                    DISORD Status ENTERED   Driving force -4.9687E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.39146E-01  B  3.60854E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01

 LRO#3                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  6.00000E-01  B  4.00000E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.98449E-01  B  1.55066E-03
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.98449E-01  B  1.55066E-03
 Sublattice  3,  Number of sites  2.5000E-01
 B  9.92271E-01  A  7.72920E-03
 Sublattice  4,  Number of sites  2.5000E-01
 B  6.04628E-01  A  3.95372E-01
POLY_3:Hit RETURN to continue
POLY_3: s-c x(b)=.33
   ... the command in full is SET_CONDITION
POLY_3: s-s-c lro *
   ... the command in full is SET_START_CONSTITUTION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    23 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=70, P=1E5, N=1., X(B)=0.33
 DEGREES OF FREEDOM 0

 Temperature     70.00 K (  -203.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -2.85605E+03,  Enthalpy -2.74060E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.7000E-01  6.7000E-01 5.7336E-02 -1.6639E+03 SER
 B                       3.3000E-01  3.3000E-01 1.1554E-04 -5.2765E+03 SER

 LRO                      ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 7.8876E-02, Mass 7.8876E-01, Volume fraction 0.0000E+00  Mole fractions:
 A  6.87496E-01  B  3.12504E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.16558E-01  B  8.34422E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.16558E-01  B  8.34422E-02
 Sublattice  3,  Number of sites  2.5000E-01
 A  9.16558E-01  B  8.34422E-02
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99689E-01  A  3.11152E-04

 LRO#2                    DISORD Status ENTERED   Driving force -4.8130E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.61498E-01  B  3.38502E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01
 Sublattice  3,  Number of sites  2.5000E-01
```

```
 A  6.61498E-01  B  3.38502E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01

 LRO#3                     ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 9.2112E-01, Mass 9.2112E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.68502E-01  B  3.31498E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.82295E-01  B  1.77045E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.82295E-01  B  1.77045E-02
 Sublattice  3,  Number of sites  2.5000E-01
 B  9.99255E-01  A  7.44800E-04
 Sublattice  4,  Number of sites  2.5000E-01
 A  7.08671E-01  B  2.91329E-01
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 2 t 0 250 5
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: save tcex31c y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: add -1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  -1  T=70, P=100000, N=1., X(B)=0.33
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: map -
 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   3.315E-01  7.000E+01
  ** LRO
     LRO#3
 *** SORRY CANNOT CONTINUE ***    4

 CALCULATED    41 EQUILIBRIA

 Phase region boundary   2 at:   3.315E-01  7.000E+01
  ** LRO
     LRO#3
 Terminating at diagram limit
 CALCULATED    68 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
 31c.POLY3
 CPU time for mapping                     1  seconds
POLY_3: @@ Add the A2/L1_2 line
POLY_3: read tcex31c
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:
POLY_3: s-c x(b)=.15 t=110
   ... the command in full is SET_CONDITION
POLY_3: s-a-s f
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    38 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=110, P=1E5, N=1., X(B)=0.15
 DEGREES OF FREEDOM 0

 Temperature    110.00 K (  -163.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -1.66707E+03,  Enthalpy -1.39975E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       8.5000E-01  8.5000E-01 7.3635E-01 -2.7991E+02 SER
 B                       1.5000E-01  1.5000E-01 2.9909E-05 -9.5277E+03 SER

 LRO                       ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 7.2552E-01, Mass 7.2552E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  8.40743E-01  B  1.59257E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.74694E-01  B  2.53056E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.74694E-01  B  2.53056E-02
 Sublattice  3,  Number of sites  2.5000E-01
 A  9.74694E-01  B  2.53056E-02
 Sublattice  4,  Number of sites  2.5000E-01
 B  5.61112E-01  A  4.38888E-01

 LRO#2                     DISORD Status ENTERED   Driving force -8.1131E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
```

```
 A  8.60606E-01  B  1.39394E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.60606E-01  B  1.39394E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.60606E-01  B  1.39394E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.60606E-01  B  1.39394E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  8.60606E-01  B  1.39394E-01

 LRO#3                    DISORD Status ENTERED   Driving force  0.0000E+00
 Moles 2.7448E-01, Mass 2.7448E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  8.74469E-01  B  1.25531E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.74469E-01  B  1.25531E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.74469E-01  B  1.25531E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.74469E-01  B  1.25531E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  8.74469E-01  B  1.25531E-01
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: map -
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

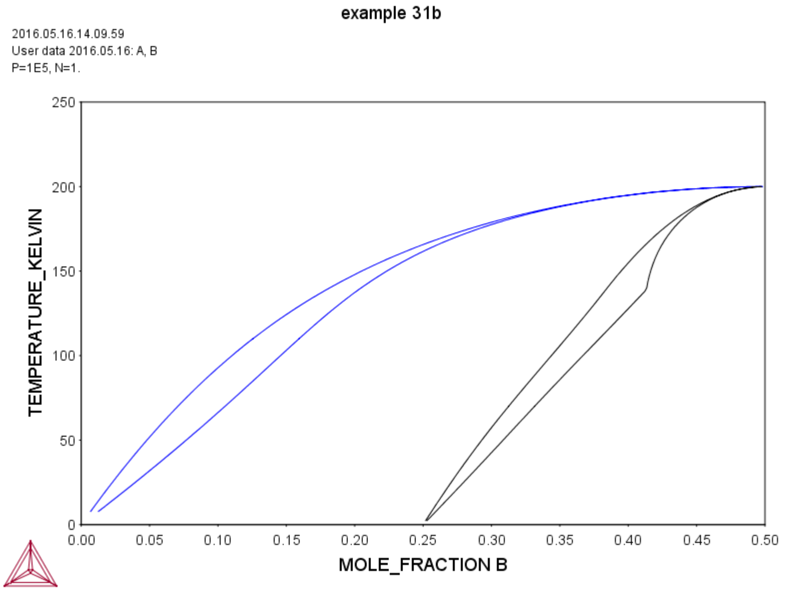
 Phase region boundary   1 at:   1.593E-01  1.100E+02
     LRO
  ** LRO#3
 MAPPING TERMINATED 1
 CALCULATED    55 EQUILIBRIA

 Phase region boundary   2 at:   1.593E-01  1.100E+02
     LRO
  ** LRO#3
 Terminating at diagram limit
 CALCULATED    69 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
 31c.POLY3
 CPU time for mapping                     0  seconds
POLY_3: post

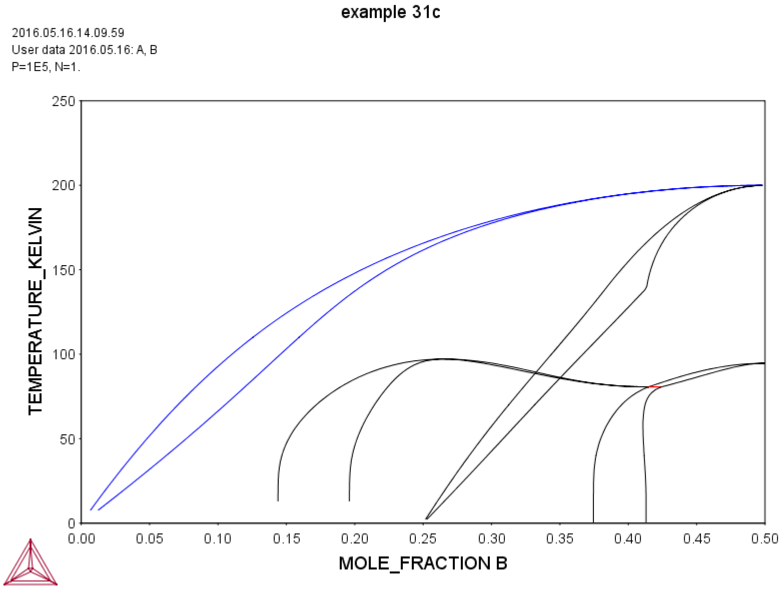
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-s x n 0 .5
   ... the command in full is SET_SCALING_STATUS
POST: @@ Usually some 2nd order lines also appear
POST: set-title example 31b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex31 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: set-title example 31c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: read tcex31c
   ... the command in full is READ_WORKSPACES
POLY_3: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: @@ Now we will add a reciprocal parameter to LRO which describes
GES: @@ the SRO contribution.  The default value of this is
GES: @@ the bond energy.  One can have 3 different such parameters
GES: @@ depending on if one is at 25%B, 50%B or 75%B.  Here we just take the
GES: @@ same value.
GES:
GES: e-sym f GSROAA,,UIJ;,,,,,
   ... the command in full is ENTER_SYMBOL
GES: e-sym f GSROAB,,UIJ;,,,,,
   ... the command in full is ENTER_SYMBOL
GES: e-sym f GSROBB,,UIJ;,,,,,
   ... the command in full is ENTER_SYMBOL
GES:
GES: e-par l(lro,a,b:a,b:*:*),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,A,B:A,B:*:*;0)
GES: e-par l(lro,a,b:*:a,b:*),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,A,B:*:A,B:*;0)
GES: e-par l(lro,a,b:*:*:a,b),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,A,B:*:*:A,B;0)
GES: e-par l(lro,*:a,b:a,b:*),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,*:A,B:A,B:*;0)
GES: e-par l(lro,*:a,b:*:a,b),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,*:A,B:*:A,B;0)
GES: e-par l(lro,*:*:a,b:a,b),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,*:*:A,B:A,B;0)
GES: l-p-d lro
   ... the command in full is LIST_PHASE_DATA


 LRO
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
   4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
     CONSTITUENTS: A,B : A,B : A,B : A,B

        G(LRO,A:A:A:A;0) = 0.0
        G(LRO,B:A:A:A;0) = +GA3B1
        G(LRO,A:B:A:A;0) = +GA3B1
        G(LRO,B:B:A:A;0) = +GA2B2
        G(LRO,A:A:B:A;0) = +GA3B1
        G(LRO,B:A:B:A;0) = +GA2B2
        G(LRO,A:B:B:A;0) = +GA2B2
        G(LRO,B:B:B:A;0) = +GA1B3
        G(LRO,A:A:A:B;0) = +GA3B1
        G(LRO,B:A:A:B;0) = +GA2B2
        G(LRO,A:B:A:B;0) = +GA2B2
        G(LRO,B:B:A:B;0) = +GA1B3
        G(LRO,A:A:B:B;0) = +GA2B2
        G(LRO,B:A:B:B;0) = +GA1B3
        G(LRO,A:B:B:B;0) = +GA1B3
        G(LRO,B:B:B:B;0) = 0.0
        L(LRO,A,B:A,B:*:*;0) = +GSROAB
        L(LRO,A,B:*:A,B:*;0) = +GSROAB
        L(LRO,A,B:*:*:A,B;0) = +GSROAB
        L(LRO,*:A,B:A,B:*;0) = +GSROAB
        L(LRO,*:A,B:*:A,B;0) = +GSROAB
        L(LRO,*:*:A,B:A,B;0) = +GSROAB
GES:
GES:Hit RETURN to continue
GES: @@ These reciprocal parameters do not give any contribution to the
GES: @@ disordered state as the contribution from the ordered phase is zero there.
GES: @@ But it is in the disordered state that the sro contribution
GES: @@ to the Gibbs energy is most important.  We must add regular solution
GES: @@ parameters to the FCC phase giving the same contribution.  These can
GES: @@ be derived by setting all site-fractions for the same element equal,
GES: @@ i.e. the disordered state.
```

```
GES: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3+
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;0)
&                     0.375*GSROAA+0.75*GSROAB+0.375*GSROBB;,,,,,
GES: e-par l(fcc,a,b;1),,2*GA3B1-2*GA1B3+0.75*GSROAA-0.75*GSROBB;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;1)
GES: e-par l(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;2)
GES: e-par l(fcc,a,b;3),,-0.75*GSROAA+0.75*GSROBB;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;3)
GES: e-par l(fcc,a,b;4),,-0.375*GSROAA+0.75*GSROAB-0.375*GSROBB;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;4)
GES: l-p-d fcc
   ... the command in full is LIST_PHASE_DATA


 FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF LRO
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
      G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
      L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3+.375*GSROAA+.75*GSROAB
           +.375*GSROBB
      L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3+.75*GSROAA-.75*GSROBB
      L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB
      L(FCC_A1,A,B;3) = -.75*GSROAA+.75*GSROBB
      L(FCC_A1,A,B;4) = -.375*GSROAA+.75*GSROAB-.375*GSROBB
GES:
GES:Hit RETURN to continue
GES: ba
   ... the command in full is BACK
POLY_3: c-st p lro#3=e 0
   ... the command in full is CHANGE_STATUS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=70, P=1E5, N=1., X(B)=0.33
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: s-c t=40
   ... the command in full is SET_CONDITION
POLY_3: s-a-s f
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    27 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=40, P=1E5, N=1., X(B)=0.33
 DEGREES OF FREEDOM 0

 Temperature     40.00 K (  -233.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -2.81177E+03,  Enthalpy -2.73484E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.7000E-01  6.7000E-01 5.5303E-03 -1.7286E+03 SER
 B                       3.3000E-01  3.3000E-01 2.8612E-07 -5.0109E+03 SER

 LRO                      ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 9.1974E-01, Mass 9.1974E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.79151E-01  B  3.20849E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  3,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99993E-01  A  6.81574E-06

 LRO#2                    DISORD Status ENTERED   Driving force -3.8166E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.26318E-01  B  3.73682E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01

 LRO#3                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 8.0263E-02, Mass 8.0263E-01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.65144E-01  B  4.34856E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.99996E-01  B  4.15407E-06
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.99996E-01  B  4.15407E-06
 Sublattice  3,  Number of sites  2.5000E-01
 B  8.69708E-01  A  1.30292E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  8.69708E-01  A  1.30292E-01
POLY_3:Hit RETURN to continue
POLY_3: save tcex31d y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
```

```
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: map -
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   3.208E-01  4.000E+01
     LRO
  ** LRO#3
 TOO LONG JUMP IN AXIS, SKIPPING NODE
 MAPPING TERMINATED 1
 CALCULATED    30 EQUILIBRIA

 Phase region boundary   2 at:   3.208E-01  4.000E+01
     LRO
  ** LRO#3
 CALCULATED    22 EQUILIBRIA

 Phase region boundary   2 at:   3.685E-01  7.734E+01
     LRO
     LRO#2
  ** LRO#3

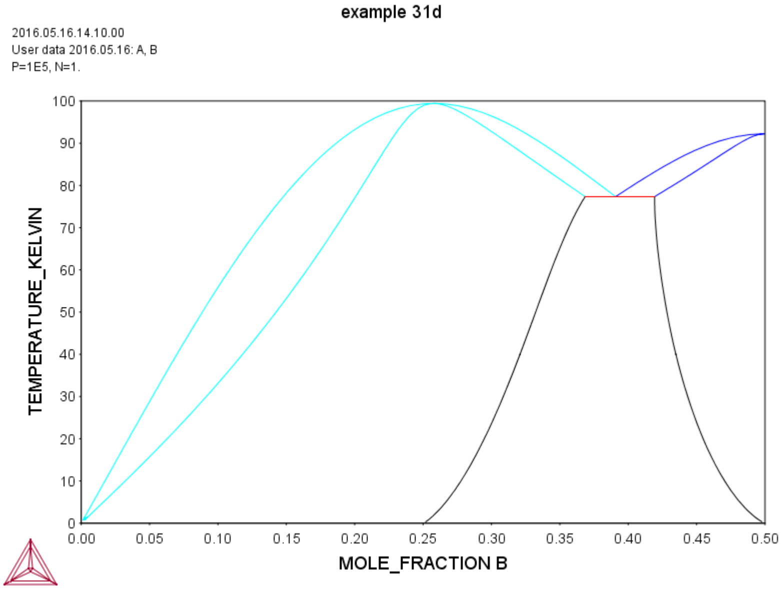
 Phase region boundary   2 at:   4.193E-01  7.734E+01
  ** LRO#2
     LRO#3
 Terminating at diagram limit
 CALCULATED    23 EQUILIBRIA

 Phase region boundary   2 at:   3.685E-01  7.734E+01
     LRO
  ** LRO#2
 Terminating at diagram limit
 CALCULATED    88 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
 31d.POLY3
 CPU time for mapping                      0  seconds
POLY_3: post

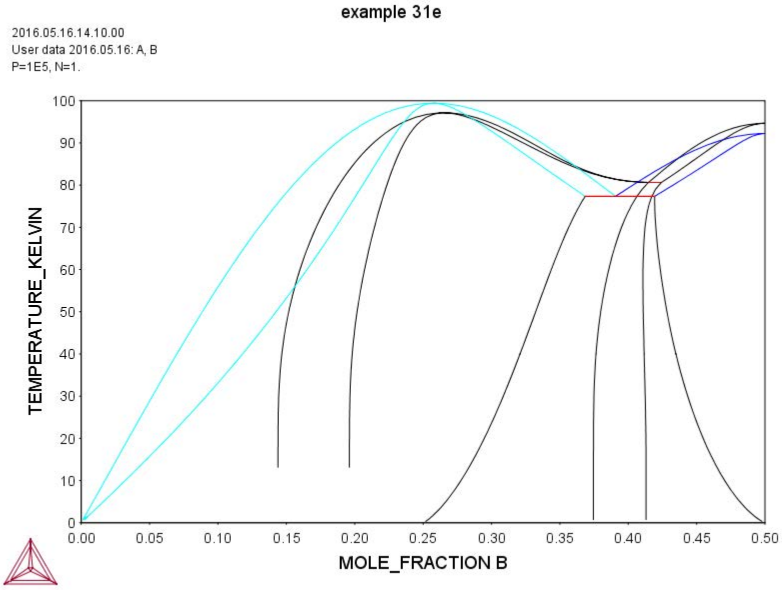
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: set-title example 31d
POST: s-s y n
   ... the command in full is SET_SCALING_STATUS
MIN VALUE : 0 100
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex31 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-title example 31e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex32

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex32\tcex32.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of oxide layers on steel
SYS: @@ and show how to append databases
SYS: @@
SYS: set-log ex32,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw tcfe7
   ... the command in full is SWITCH_DATABASE
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE7: d-sys fe cr c v mn si
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
 V                       MN                      SI
   DEFINED
TDB_TCFE7: rej ph /all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M5C2                    M3C2
 MC_ETA                  KSI_CARBIDE             A1_KAPPA
 KAPPA                   Z_PHASE                 FE4N_LP1
 FECN_CHI                SIGMA                   CHI_A12
 LAVES_PHASE_C14         M3SI                    G_PHASE
 CR3SI                   FE2SI                   MSI
 M5SI3                   AL4C3                   FE8SI2C
 SIC  REJECTED
TDB_TCFE7: rest ph fcc_a1 bcc_a2 hcp_a3 m23 m7 cementite
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  HCP_A3
 M23C6                   M7C3                    CEMENTITE
   RESTORED
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;
      Fe-Si and Fe-Si-C'
  'W. Huang, TRITA-MAC 431 (1990); C-V'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, Metall. Trans. A, 24A (1993), 1919-1933; Cr-Mn, Fe-Cr-Mn'
  'B.-J. Lee, KRISS, unpublished research, during 1993-1995'
  'B.-J. Lee, TRITA-MAC 474 (1991); Cr-Fe-V'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'W. Huang, TRITA-MAC 432 (Rev 1989,1990); FE-V'
  'J-O. Andersson, Calphad, 7 (1983), 305-315 (parameters revised 1986 due
      to new decription of V) TRITA 0201 (1982); FE-V'
  'J.E. Tibballs, SI Norway (1991) Rep. 890221-5; Mn-Si'
  'W. Huang, TRITA-MAC 439 (1990); Mn-V, Fe-Mn-V *'
  'M.H. Rand and N. Saunders, COST 507 Report (1998); Si-V'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'B.-J. Lee, Metall. Trans. A, 24A (1993), 1017-1025; Fe-Cr-Mn-C'
  'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe
      -Si-C'
  'W. Huang, TRITA-MAC 432 (1990); C-Fe-V'
  'A. Fernandez Guillermet and W. Huang, TRITA-MAC 440 (1990); Mn-V-C *'
  'A. Forsberg and J. Agren, J. Phase Equil., 14 (1993), 354-363; Fe-Mn-Si'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
      M23C6'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-V-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
  'Unassessed parameter'
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'K. Frisk, Calphad, 17 (1993), 335-349; Cr-Mn-N'
  'W. Huang, TRITA-MAC 441 (1990); Fe-Mn-V-C'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'B.-J. Lee, TRITA-MAC 475 (1991); C-Cr-Fe-V'
  'C. Qiu, Metall. Trans. A, 24A (1993), 2393-2409; Cr-Fe-Mn-N'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
```

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  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
  'Thermo-Calc Software (2008): Volume data updated for TCFE6 database (TCFE
      v6, April, 2008).'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, Vol.
      53, pp. 105-125; Molar volumes'
 -OK-
TDB_TCFE7: @@ All oxides from the substance database
TDB_TCFE7: app ssub5
   ... the command in full is APPEND_DATABASE
 Current database: SGTE Substances Database v5.1

 VA  DEFINED
APP:
APP: d-sys fe cr v si mn o c
   ... the command in full is DEFINE_SYSTEM
 FE                       CR                       V
 SI                       MN                       O
 C  DEFINED
APP: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
      C1<G> C<G>
   C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      C1O1<G> CO<G>
      CARBON MONOXIDE <GAS>
      STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
   C1O2<G> T.C.R.A.S. Class: 2
      C1O2<G> CO2<G>
      CARBON DIOXIDE <GAS>
   C1SI1<G> T.C.R.A.S. Class: 5
      C1SI1<G> SiC<G>
      SILICON CARBIDE <GAS>
   C1SI2<G> T.C.R.A.S. Class: 6
      C1SI2<G> Si2C<G>
      DISILICON CARBIDE <GAS>
   C1SI3<G> THERMODATA 02/94 BC
      C1SI3<G> Si3C<G>
   C1SI4<G> THERMODATA 02/94 BC
      C1SI4<G> Si4C<G>
   C2<G> T.C.R.A.S. Class: 2
      C2<G>
      CARBON Diatomic Gas.
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      C2O1<G> C2O<G>
   C2SI1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      C2SI1<G> SiC2<G>
      PUBLISHED BY JANAF AT 3/67
   C2SI2<G> THERMODATA 02/94 BC
      C2SI2<G> Si2C2<G>
   C2SI3<G> THERMODATA 03/94 BC
      C2SI3<G> Si3C2<G>
   C3<G> T.C.R.A.S. Class: 6
      C3<G>
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   C3O2<G> T.C.R.A.S. Class: 6
      C3O2<G>
   C4<G> T.C.R.A.S. Class: 7
      C4<G>
   C5<G> T.C.R.A.S. Class: 7
      C5<G>
   C5FE1O5<G> JANAF 1982 SGTE
      C5FE1O5<G> Fe(CO)5<G>
      IRON PENTACARBONYL <GAS>
      ASSESSMENT DATED 3/78
   C60<G> MHR-95
      C60<G>
      Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
      J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the rotational
      data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that
      a frequency with degeneracy 5 is missing from list in [94Kor/Sid];
      taken to be 419 cm-1, which gives very good, though not exact,
      agreement with values quoted in [94Kor/Sid]. Note discrepancy
      between calculated DrS(298) = -8943.5 J mol K-1 for the reaction
      60C<g>=C60<g>and that given by [94Kor/Sid] in their Table 5,
      -8950 J mol K-1. Enthalpy of formation: DfH = 2588 kJ/mol from
      DsubH(298.15K) = 166 +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure
      values reproduced very well.
      [91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).
   CR1<G> THERMODATA
      CR1<G> Cr<G>
      New Assessment (H_form and S only)
   CR1O1<G> T.C.R.A.S. Class: 5
      CR1O1<G> CrO<G>
   CR1O2<G> T.C.R.A.S. Class: 6
      CR1O2<G> CrO2<G>
      CHROMIUM DIOXIDE <GAS>
   CR1O3<G> T.C.R.A.S. Class: 6
      CR1O3<G> CrO3<G>
      CHROMIUM TRIOXIDE <GAS>
   CR2<G> THERMODATA
      CR2<G> Cr2<G>
      New assessment (H_form and S only)
   CR2O1<G> T.C.R.A.S. Class: 6
      CR2O1<G> Cr2O<G>
   CR2O2<G> T.C.R.A.S. Class: 6
      CR2O2<G> Cr2O2<G>
   CR2O3<G> T.C.R.A.S. Class: 7
      CR2O3<G> Cr2O3<G>
      CHROMIUM<3> OXIDE <GAS>
   FE1<G> THERMODATA
      FE1<G> Fe<G>
```

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   Data provided by T.C.R.A.S. October 1996
   Modified by Thermodata - new assessment
FE1O1<G> TCRAS 5-F FEO IRON OXIDE 23/11/06
   FE1O1<G> FeO<G>
FE1O2<G> T.C.R.A.S Class: 6
   FE1O2<G> FeO2<G>
   Data provided by TCRAS. October 1996. Error in version 1997.
   S298 corrected to 1bar
   20080222 AAZ TCRAS2006 : dH, S
FE2<G> THERMODATA
   FE2<G> Fe2<G>
   Data provided by T.C.R.A.S. October 1996
   Modified by Thermodata - new assessment.
   Typing error corrected 12/06
MN1<G> THERMODATA 01/93
   MN1<G> Mn<G>
   MANGANESE <GAS>
   28/01/93
MN1O1<G> T.C.R.A.S. Class: 2
   MN1O1<G> MnO<G>
   MANGANESE<2> OXIDE <GAS>
MN1O2<G> T.C.R.A.S. Class: 7
   MN1O2<G> MnO2<G>
   MANGANESE<4> OXIDE <GAS>
O1<G> TCRAS 02/06/80
   O1<G> O<G>
O10V4<G> T.C.R.A.S. Class: 7
   O10V4<G> V4O10<G>
O1SI1<G> T.C.R.A.S. Class: 1
   O1SI1<G> SiO<G>
   SILICON <MONOXIDE GAS>
O1V1<G> T.C.R.A.S. Class: 5
   O1V1<G> VO<G>
   VANADIUM MONOXIDE <GAS>
O2<G> TCRAS 21/06/90
   O2<G>
   OXYGEN Gaseous Standard State.
O2SI1<G> T.C.R.A.S. Class: 5
   O2SI1<G> SiO2<G>
   SILICON DIOXIDE <GAS>
O2SI2<G> CHATILLON(1995)
   O2SI2<G> Si2O2<G>
   Hf from mass spectrometry Zmbov K.F., Ames L.L., Margrave J.L., High
   Temp. Sci. 5 (1973)235 and Rocabois Ph., Chatillon C. , Bernard. C.
   Rev. Int. Hautes Temper. Refract. Fr. 28 (1992-93) 37-48 and Cp, S(T)
   an
   Fef from Al2O2<G> according to Al2O2 by Dimensional Model (Frurip and Bl
O2V1<G> T.C.R.A.S. Class: 5
   O2V1<G> VO2<G>
   VANADIUM DIOXIDE <GAS>
O3<G> TCRAS 02/06/80
   O3<G>
   OZONE Gaseous Standard State.
SI1<G> T.C.R.A.S. Class: 1
   SI1<G> Si<G>
   SILICON <GAS>
SI2<G> T.C.R.A.S. Class: 5
   SI2<G> Si2<G>
   SILICON <DIATOMIC GAS>
SI3<G> T.C.R.A.S. Class: 6
   SI3<G> Si3<G>
   SILICON <TRIATOMIC GAS>
V1<G> T.C.R.A.S. Class: 1
   V1<G> V<G>
   VANADIUM <GAS>
O2SI1<BETA-QUARTZ> N.P.L.
   O2SI1_BETA_QUARTZ SiO2_BETA_QUARTZ
   Data from an assessment by T I Barry, reported in paper on CaO-SiO2
   system by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
C0.88V1 THERMODATA 01/93
   C0.88V1 VC0.88
   28/01/93
C1FE1O3 N.P.L. SGTE **
   C1FE1O3 FeCO3 Siderite
   IRON<2> CARBONATE
   DECOMPOSES BEFORE FUSION.
C1FE3 N.P.L. SGTE **
   C1FE3 Fe3C Cementite
   CEMENTITE
C1MN1O3 KUBASCHEWSKI EVANS ALCOCK 1967 SGTE **
   C1MN1O3 MnCO3
   MANGANESE<2> CARBONATE
C1MN3 M. ANCEY, Y. DENIEL SGTE
   C1MN3 Mn3C
   TRIMANGANESE MONOCARBIDE
C1SI1<C1SI1_ALPHA> JANAF THERMOCHEMICAL TABLES SGTE **
   C1SI1_ALPHA SiC_ALPHA
   N CARBIDE <ALPHA>
   ALPHA-SIC . HEX.FORM . PUBL. BY JANAF AT 3/67 .LESS STABLE THAN
   SIC_BETA UP TO 2200K. Decomposes to complex vapour at about 3259K.
C1SI1<C1SI1_BETA> JANAF THERMOCHEMICAL TABLES SGTE
   C1SI1_BETA SiC_BETA
   N CARBIDE <BETA>
   CUBIC FORM OF TYPE ZNS. STABLE WITH RESPECT TO SIC-ALPHA UP TO 2200K.
   PUBL. BY JANAF 03/67
C1V2 THERMODATA 01/93
   C1V2 V2C
   DIVANADIUM MONOCARBIDE
   28/01/93 Tm=2438 K.
C2CR3 JANAF THERMOCHEMICAL TABLES SGTE
   C2CR3 Cr3C2
   3-CHROMIUM 2-CARBIDE
   (1975 SUPPL.) PUBLISHED BY JANAF AT 12/73
   Melts incongruently at 2168K.
C2MN5 T.C.R.A.S. Class: 7
   C2MN5 Mn5C2
C3CR7 JANAF THERMOCHEMICAL TABLES SGTE **
   C3CR7 Cr7C3
   7-CHROMIUM 3-CARBIDE
   PUBLISHED BY JANAF AT 12/73 .REVISED VALUE FOR DELTA H 298
   BY B.UHRENIUS 1980 Melts incongruently at 2053K.
C3MN7 S.G.T.E. SGTE **
   C3MN7 Mn7C3
   HEPTAMANGANESE TRICARBIDE
   REASSESMENT BY B.URHENIUS
C5FE1O5<L> I. BARIN 3rd. Edition
```

```
   C5FE1O5_Liquid Fe(CO)5_Liquid
   IRON PENTACARBONYL (Liquid). Same as in previous versions.
   Rounding of H298.
C60 MHR-95
   C60
   Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.
   The
   Fitted to the data in [94Kor/Sid], who took the phase transition at
   257K
   that [94Kor/Sid] do not give an explicit value for S(298.15K).
   S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =425.8 and Cp
   e
   calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]
   in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.
   Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
   the value preferred, if obliquely, by [94Kor/Sid].
   [92Ste/Chi]W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,
   P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).
C6CR1O6 I. BARIN 3rd. Edition
   C6CR1O6 Cr(CO)6
   CHROMIUM HEXACARBONYL
   SUBLIMATION AT 424K.
C6CR23 JANAF THERMOCHEMICAL TABLES SGTE
   C6CR23 Cr23C6
   23-CHROMIUM 6-CARBIDE
   ((1975 SUPPL.)) PUBLISHED BY JANAF AT 12/73
   Melts incongruently at 1793K.
C6MN23 T.C.R.A.S. Class: 7
   C6MN23 Mn23C6
CR1O2 S.G.T.E. SGTE **
   CR1O2 CrO2
   CHROMIUM DIOXIDE
   O.KUBASCHEWSKI'S REASSESSMENT 1979
CR1O3 S.G.T.E. SGTE **
   CR1O3 CrO3
   CHROMIUM TRIOXIDE
   O.KUBASCHEWSKI'S REASSESSMENT 1979
CR1SI1 T.C.R.A.S. Class: 6
   CR1SI1 CrSi
   CHROMIUM SILICON
CR1SI2 T.C.R.A.S. Class: 7
   CR1SI2 CrSi2
   CHROMIUM 2-SILICON
CR2FE1O4 KUBASCHEWSKI EVANS ALCOCK 1967 SGTE
   CR2FE1O4 FeCr2O4 FeO-Cr2O3
   DELTAH 298 CALCULATED FROM OXIDES =-13100CAL/MOL(#1000)
CR2O3 T.C.R.A.S. Class: 7
   CR2O3 Cr2O3
   CHROMIUM<3> OXIDE
   cp refitted by AP because of low T FC at 306K
CR3SI1 T.C.R.A.S. Class: 7
   CR3SI1 Cr3Si
   3-CHROMIUM 2-SILICON
CR5O12 S.G.T.E. SGTE **
   CR5O12 Cr5O12
   5-CHROMIUM 12-OXIDE
   CR5O12: 5-CHROMIUM 12-OXIDE **DECOMPOSITION (643 -->705 K)
   O.KUBASCHEWSKI'S REASSESSMENT 1979.
CR5SI3 T.C.R.A.S. Class: 7
   CR5SI3 Cr5Si3
   5-CHROMIUM 3-SILICON
CR8O21 S.G.T.E. SGTE **
   CR8O21 Cr8O21
   8-CHROMIUM 21-OXIDE
   O.KUBASCHEWSKI'S REASSESSMENT 1971
   CR8O21 8-CHROMIUM 21-OXIDE,DECOMPOSITION (600 --> 640K.)
O2SI1<CRISTOBALITE> N.P.L.
   O2SI1_CRISTOBALITE SiO2_CRISTOBALITE
   Data from an assessment by T I Barry, reported in paper on CaO-SiO2
   syst
   by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
CR1 S.G.T.E. **
   CR1 Cr
   Data from SGTE Unary DB
C1<DIAMOND> S.G.T.E. **
   C_DIAMOND
   <DIAMOND>
   Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
   from 1994 database (ex THERMODATA 01/93)
FE2O4SI1<FAYALITE> S.G.T.E.
   FE2O4SI1 Fe2SiO4 FAYALITE 2FeO-SiO2
   IRON ORTHOSILICATE <FAYALITE>
   Data assessed by M. Selleby. 20/5/94
FE1O1 T.C.R.A.S Class: 5
   FE1O1 FeO FeO_Wustite
   IRON OXIDE. Data provided by T.C.R.A.S. in 2000
FE1O3SI1 THERMODATA 01/93
   FE1O3SI1 FeSiO3 FeO-SiO2
   28/01/93
FE1O4V2 THERMODATA 01/93
   FE1O4V2 FeV2O4 FeO-V2O3
   28/01/93
FE1O6V2 THERMODATA 01/93
   FE1O6V2 FeV2O6 FeO-V2O5
   IRON VANADATE
   28/01/93 Td = 1023 K.
FE1SI1 THERMODATA 01/93
   FE1SI1 FeSi
   IRON SILICIDE
   28/01/93
FE1SI2.33 THERMODATA 01/93
   FE1SI2.33 FeSi2.33
   LEBOITE <ALPHA>
   28/01/93 LEBOITE (ALPHA).
FE1SI2 THERMODATA 01/93
   FE1SI2 FeSi2
   LEBOITE <BETA>
   28/01/93 LEBOITE (BETA). Td = 1243K
FE2MN1O4 O. KUBASCHEWSKI DCS REPORT 7 . SGTE
   FE2MN1O4 MnFe2O4 MnO-Fe2O3
   MANGANESE DIIRON TETRAOXIDE
   BARIN
   KNACKE ED 73 REF *,5,1 (KUBASCHEWSKI) .
FE2O3<FE2O3_GAMMA> T.C.R.A.S Class: 5
   FE2O3_GAMMA Fe2O3_Gamma
   Data provided by T.C.R.A.S. in 2000
```

```
   FE1 S.G.T.E. **
      FE1 Fe
      Data from SGTE Unary DB
   C1<GRAPHITE> S.G.T.E. **
      C_GRAPHITE
      Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
   FE2O3<HEMATITE> T.C.R.A.S Class: 7
      FE2O3 Fe2O3 Hematite
      Data provided by T.C.R.A.S. in 2000 with previous description
      of the magnetic transition fitted by IA. In version 2000 only
      H298 has been changed.
   FE3O4<MAGNETITE> JANAF 4th Ed.
      FE3O4 Fe3O4 MAGNETITE
      Data refitted by IA to reproduce the magnetic transition.
   MN11SI19 N.P.L. FEB. 1994
      MN11SI19 Mn11Si19
   MN1O1 I. BARIN 3rd. Edition
      MN1O1 MnO
      MANGANESE OXIDE.Data taken from BARIN 3rd. Ed. (1995)
   MN1O2 I. BARIN 3rd. Edition
      MN1O2 MnO2
      MANGANESE<4> OXIDE. Data taken from BARIN 3rd. Ed. (1995).
      S(298) FROM N.P.L.
   MN1SI1 T.G. CHART NPL REPORT.CHEM.18 AUGUST 197 SGTE
      MN1SI1 MnSi
      MANGANESE SILICON
      S(298.15) CALCULATED FROM CHART'S PUBLISHED VALUE FOR DELTA S(298.15)
      FORMATION AND HULTGREN'S DATA OF S(298.15) FOR SI AND CR (REF.4)
   MN2O3 KUBASCHEWSKI EVANS ALCOCK 1967 SGTE **
      MN2O3 Mn2O3
      MANGANESE<3> OXIDE
      DATA CORRESPONDS TO MNO1.5-1.6. DECOMPOSITION BEFORE MELTING.
   MN2O7<L> T.C.R.A.S. Class: 7
      MN2O7 Mn2O7
   MN3O4 KUBASCHEWSKI DCS REPORT 7 . SGTE
      MN3O4 Mn3O4 MnO-Mn2O3
      MANGANESE<2,3> OXIDE
      MNO(1.33-1.41) .
   MN3SI1 N.P.L. FEB. 1994
      MN3SI1 Mn3Si
      3-MANGANESE SILICON
   MN4SI7 T.G. CHART NPL REPORT.CHEM.18 AUG 1997 SGTE
      MN4SI7 Mn4Si7
      S(298.15) CALCULATED FROM CHART'S PUBLISHED VALUE FOR DELTA S(298.15)
      FORMATION AND HULTGREN'S DATA OF S(298.15) FOR SI AND CR (REF.4)
   MN5SI3 T.G. CHART NPL REPORT.CHEM.18 AUG 1997 SGTE
      MN5SI3 Mn5Si3
      5-MANGANESE 3-SILICON
      S(298.15) CALCULATED FROM CHART'S PUBLISHED VALUE FOR DELTA S(298.15)
      FORMATION AND HULTGREN'S DATA OF S(298.15) FOR SI AND CR (REF.4)
   MN1 S.G.T.E. **
      MN1 Mn
      Data from SGTE Unary DB
   O1V1 T.C.R.A.S. Class: 6
      O1V1 VO
      VANADIUM MONOXIDE
   O3V2 T.C.R.A.S. Class: 6
      O3V2 V2O3
      VANADIUM TRIOXIDE
   O4V2 T.C.R.A.S. Class: 7
      O4V2 V2O4<G> (VO2)2<G>
   O5V2 T.C.R.A.S. Class: 7
      O5V2 V2O5
      VANADIUM PENTOXIDE
   O2SI1<QUARTZ> N.P.L.
      O2SI1_QUARTZ SiO2_Quartz SiO2_Alpha_Quartz
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   MN1O3SI1<RHODONITE> I. BARIN 3rd. Edition
      MN1O3SI1 MnSiO3 RHODONITE MnO-SiO2
      MANGANESE METASILICATE <RHODONITE> .Data taken from BARIN 3rd.
      Ed. (1995)
   SI1V3 THERMODATA 10/85 BC
      SI1V3 SiV3
   SI2V1 T.G. CHART NPL REPORT.CHEM.18 AUGUST 197 SGT
      SI2V1 VSi2
      VANADIUM 2-SILICON
      S(298.15) CALCULATED FROM CHART'S PUBLISHED VALUE FOR DELTA S(298.15)
      FORMATION AND HULTGREN'S DATA OF S(298.15) FOR SI AND CR (REF.4)
   SI3V5 THERMODATA 10/85
      SI3V5 V5Si3
   O2SI1<SIO2_LIQUID> N.P.L.
      O2SI1_LIQUID SiO2_Liquid
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   SI1 JANAF THERMOCHEMICAL TABLES SGTE **
      SI1 Si
      SILICON
      PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
      --U.D. 31/10/85
   MN2O4SI1<TEPHROITE> I. BARIN 3rd. Edition
      MN2O4SI1 Mn2SiO4 TEPHROITE 2MnO-SiO2
      MANGANESE ORTHOSILICATE <TEPHROITE>. H298, S298 and Tmax modified
   O2SI1<TRIDYMITE> N.P.L.
      O2SI1_TRIDYMITE SiO2_TRIDYMITE
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   V1 S.G.T.E. **
      V1 V
      VANADIUM
      Data from SGTE Unary DB
   FE0.947O1<WUSTITE> T.C.R.A.S Class: 5
      FE0.947O1 Fe0.947O WUSTITE
      WUSTITE. Data provided by T.C.R.A.S. in 2000
      20080222 AAZ TCRAS2006 : dH, S
 -OK-
APP: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3:
POLY_3: s-c b(cr)=16 b(v)=.1 b(c)=1 b(mn)=.3 b(si)=.3 t=1073 p=1e5 b=100
   ... the command in full is SET_CONDITION
```

```
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100
 DEGREES OF FREEDOM 1
POLY_3:
POLY_3: @@set-start-value y(fcc_a1#2,si)=1e-2
POLY_3: @@set-start-value y(fcc_a1#1,si)=1e-12
POLY_3: set-start-const fcc#1
   ... the command in full is SET_START_CONSTITUTION
Y(FCC_A1,CR) /1/: 1e-6
Y(FCC_A1,FE) /1/: 0.999
Y(FCC_A1,MN) /1/: 4e-6
Y(FCC_A1,SI) /1/: 1e-9
Y(FCC_A1,V) /1/: 5e-7
Y(FCC_A1,C#2) /1/: 4e-2
Y(FCC_A1,VA#2) /1/: 0.96
POLY_3: set-start-const fcc#2
   ... the command in full is SET_START_CONSTITUTION
Y(FCC_A1#2,CR) /1/: 2e-2
Y(FCC_A1#2,FE) /1/: 0.4
Y(FCC_A1#2,MN) /1/: 7e-4
Y(FCC_A1#2,SI) /1/: 4e-4
Y(FCC_A1#2,V) /1/: 0.6
Y(FCC_A1#2,C#2) /1/: 0.8
Y(FCC_A1#2,VA#2) /1/: 0.2
POLY_3:Hit RETURN to continue
POLY_3: @@ We have atomic oxygen as component, later we will use
POLY_3: @@ the partial pressure of o2 as output. The state variable LNACR is
POLY_3: @@ the chemical potential divided by RT, usual values are between -40 and 0
POLY_3: s-c lnacr(o)=-27
   ... the command in full is SET_CONDITION
POLY_3: s-r-s o gas * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          9034 grid points in              0 s
   135 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB5

 Conditions:
 B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100,
    LNACR(O)=-27
 DEGREES OF FREEDOM 0

 Temperature   1073.00 K (   799.85 C),  Pressure  1.000000E+05
 Number of moles of components  2.23269E+00,  Mass in grams  1.00000E+02
 Total Gibbs energy -2.78602E+05,  Enthalpy -1.28388E+05,  Volume  9.84603E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       8.3257E-02  1.0000E-02 1.9687E-01 -1.4499E+04 SER
 CR                      3.0772E-01  1.6000E-01 5.3299E-06 -1.0833E+05 SER
 FE                      1.3332E+00  7.4453E-01 4.8257E-03 -4.7585E+04 SER
 MN                      5.4607E-03  3.0000E-03 1.0592E-07 -1.4328E+05 SER
 O                       4.9044E-01  7.8466E-02 1.8795E-12 -2.4088E+05 GAS
 SI                      1.0681E-02  3.0000E-03 7.4765E-14 -2.6965E+05 SER
 V                       1.9631E-03  1.0000E-03 2.9371E-08 -1.5473E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.3878E+00, Mass 7.5134E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  9.90936E-01  CR  3.05125E-04  V   6.34556E-05  O   0.00000E+00
 C   8.62498E-03  MN  7.05949E-05  SI  1.76803E-07

 CR2O3_S                     Status ENTERED     Driving force  0.0000E+00
 Moles 7.6819E-01, Mass 2.3351E+01, Volume fraction 0.0000E+00  Mass fractions:
 CR  6.84207E-01  C   0.00000E+00  MN  0.00000E+00  V   0.00000E+00
 O   3.15793E-01  SI  0.00000E+00  FE  0.00000E+00

 TEPHROITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.8775E-02, Mass 5.4167E-01, Volume fraction 0.0000E+00  Mass fractions:
 MN  5.44054E-01  SI  1.39069E-01  V   0.00000E+00  CR  0.00000E+00
 O   3.16878E-01  C   0.00000E+00  FE  0.00000E+00

 BETA_QUARTZ                 Status ENTERED     Driving force  0.0000E+00
 Moles 2.3997E-02, Mass 4.8061E-01, Volume fraction 0.0000E+00  Mass fractions:
 O   5.32554E-01  C   0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
 SI  4.67446E-01  V   0.00000E+00  FE  0.00000E+00

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 2.9304E-02, Mass 3.5197E-01, Volume fraction 0.0000E+00  Mass fractions:
 C   1.00000E+00  SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
 V   0.00000E+00  O   0.00000E+00  FE  0.00000E+00

 O3V2_S                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.6737E-03, Mass 1.4010E-01, Volume fraction 0.0000E+00  Mass fractions:
 V   6.79762E-01  C   0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
 O   3.20238E-01  SI  0.00000E+00  FE  0.00000E+00
POLY_3: sh lnacr(o)
   ... the command in full is SHOW_VALUE
 LNACR(O)=-27
POLY_3: @@ List also the activity of O2
POLY_3: show lnacr(o2,gas)
   ... the command in full is SHOW_VALUE
 LNACR(O2,GAS)=-54
POLY_3:Hit RETURN to continue
POLY_3: @@ Vary the normalized chemical potential of oxygen between -20 and -40
POLY_3: s-a-v 1 lnacr(o)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: -40
Max value /1/: -20
Increment /.5/: 0.25
POLY_3: save tcex32 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
 No initial equilibrium, using default
 Step will start from axis value   -27.0000
...OK
```

```
Phase Region from   -27.0000     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1
    GRAPHITE
    O3V2_S
    TEPHROITE
Global check of adding phase at -2.66392E+01
Calculated     4 equilibria

Phase Region from   -26.6392     for:
    BETA_QUARTZ
    CR2FE1O4_S
    CR2O3_S
    FCC_A1
    GRAPHITE
    O3V2_S
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -26.6392     for:
    BETA_QUARTZ
    CR2FE1O4_S
    FCC_A1
    GRAPHITE
    O3V2_S
    TEPHROITE
Global check of adding phase at -2.48680E+01
Calculated    10 equilibria

Phase Region from   -24.8680     for:
    BETA_QUARTZ
    CR2FE1O4_S
    FCC_A1
    FE1O4V2_S
    GRAPHITE
    O3V2_S
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -24.8680     for:
    BETA_QUARTZ
    CR2FE1O4_S
    FCC_A1
    FE1O4V2_S
    GRAPHITE
    TEPHROITE
Global check of adding phase at -2.32956E+01
Calculated     9 equilibria

Phase Region from   -23.2956     for:
    GAS
    BETA_QUARTZ
    CR2FE1O4_S
    FCC_A1
    FE1O4V2_S
    GRAPHITE
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -23.2956     for:
    GAS
    BETA_QUARTZ
    CR2FE1O4_S
    FCC_A1
    FE1O4V2_S
    TEPHROITE
Global check of adding phase at -2.30914E+01
Calculated     4 equilibria

Phase Region from   -23.0914     for:
    GAS
    BETA_QUARTZ
    CR2FE1O4_S
    FAYALITE
    FCC_A1
    FE1O4V2_S
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -23.0914     for:
    GAS
    CR2FE1O4_S
    FAYALITE
    FCC_A1
    FE1O4V2_S
    TEPHROITE
Global check of adding phase at -2.28036E+01
Calculated     4 equilibria

Phase Region from   -22.8036     for:
    GAS
    CR2FE1O4_S
    FAYALITE
    FCC_A1
    FE1O1_S
    FE1O4V2_S
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -22.8036     for:
    GAS
    CR2FE1O4_S
    FAYALITE
    FE1O1_S
    FE1O4V2_S
    TEPHROITE
Global test at -2.10000E+01 .... OK
Terminating at   -20.0000
Calculated    15 equilibria

Phase Region from   -27.0000     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1
```

```
    GRAPHITE
    O3V2_S
    TEPHROITE
Global check of adding phase at -2.78680E+01
Calculated     6 equilibria

Phase Region from   -27.8680     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1
    FCC_A1#2
    GRAPHITE
    O3V2_S
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -27.8680     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1
    FCC_A1#2
    GRAPHITE
    TEPHROITE
Global check of adding phase at -2.82727E+01
Calculated     5 equilibria

Phase Region from   -28.2727     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1
    FCC_A1#2
    GRAPHITE
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -28.2727     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1
    FCC_A1#2
    TEPHROITE
Global check of adding phase at -2.95967E+01
Calculated     8 equilibria

Phase Region from   -29.5967     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1
    FCC_A1#2
    M7C3
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -29.5967     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1
    M7C3
    TEPHROITE
Global check of removing phase at -2.96631E+01
Calculated     3 equilibria

Phase Region from   -29.6631     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1
    M7C3
    TEPHROITE
Global check of adding phase at -3.04150E+01
Calculated     6 equilibria

Phase Region from   -30.4150     for:
    BCC_A2
    BETA_QUARTZ
    CR2O3_S
    FCC_A1
    M7C3
    TEPHROITE
Global check of removing phase at -3.04211E+01
Calculated     3 equilibria

Phase Region from   -30.4211     for:
    BCC_A2
    BETA_QUARTZ
    CR2O3_S
    M7C3
    TEPHROITE
Global check of removing phase at -3.10968E+01
Calculated     6 equilibria

Phase Region from   -31.0968     for:
    BCC_A2
    BETA_QUARTZ
    M7C3
    TEPHROITE
Global check of removing phase at -3.12857E+01
Calculated     4 equilibria

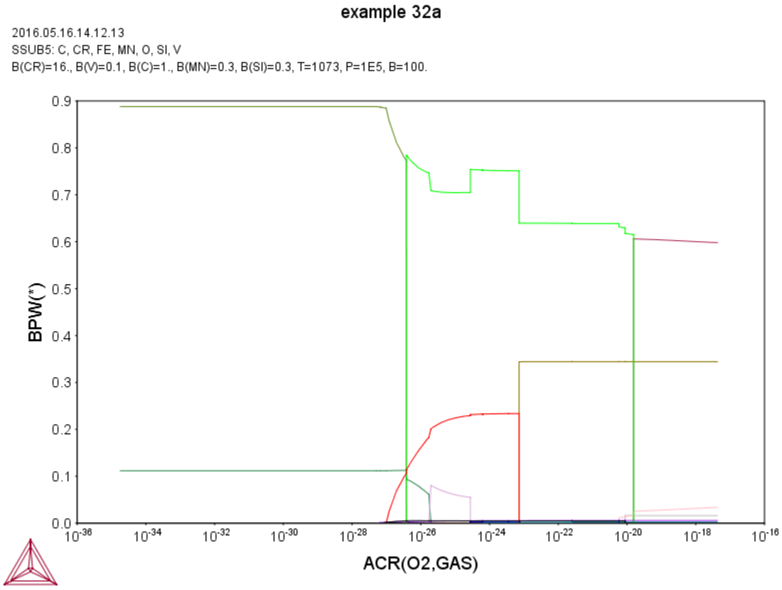
Phase Region from   -31.2857     for:
    BCC_A2
    M7C3
    TEPHROITE
Global check of removing phase at -3.14255E+01
Calculated     3 equilibria

Phase Region from   -31.4255     for:
    BCC_A2
    M7C3
Global test at -3.32500E+01 .... OK
Global test at -3.57500E+01 .... OK
Global test at -3.82500E+01 .... OK
Terminating at   -40.0000
```

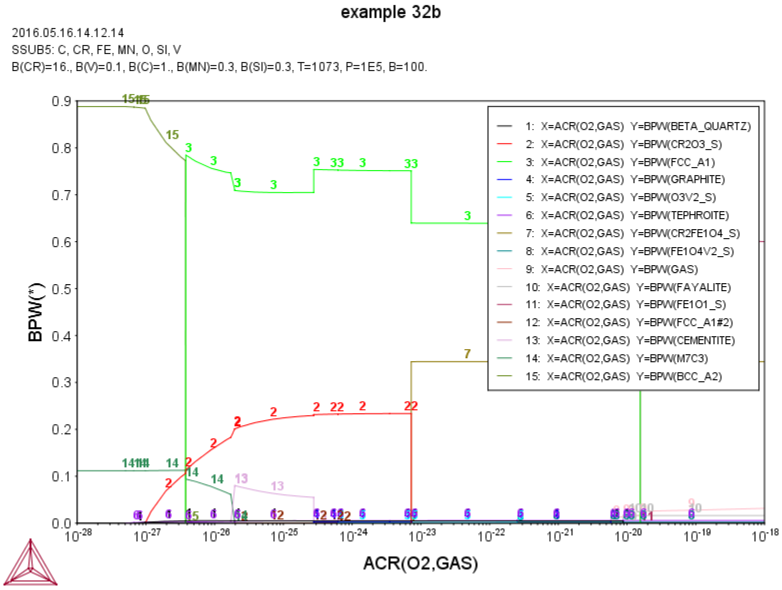
```
 Calculated    38 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex32\tcex
 32.POLY3
POLY_3:
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2

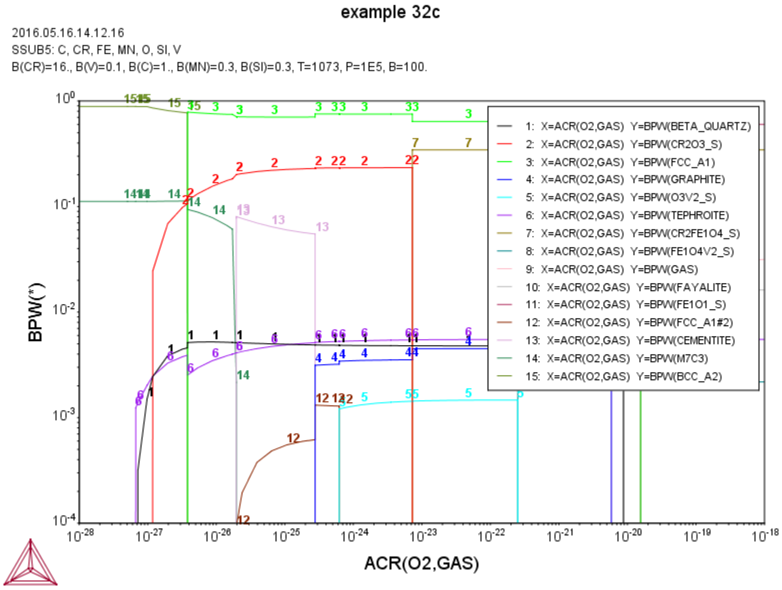
POST:
POST: s-d-a x acr(o2,gas)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y bpw(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-a-ty
   ... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST: set-title example 32a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



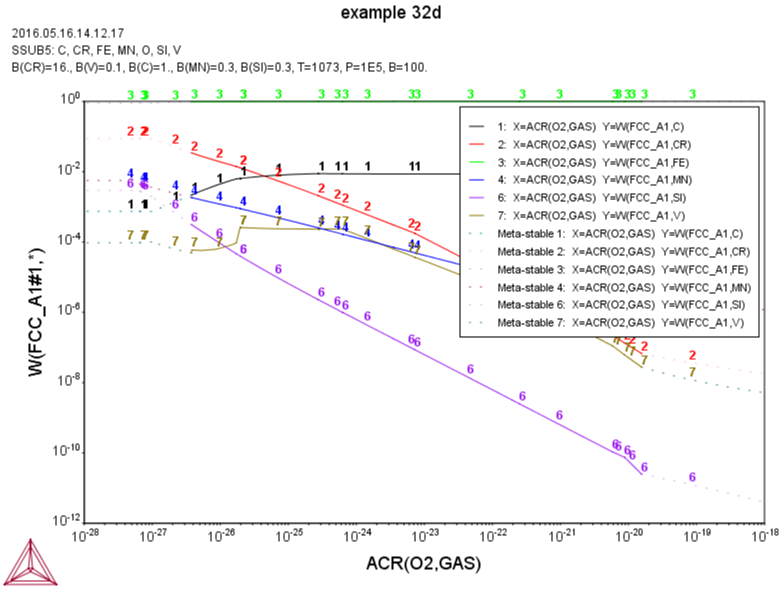
```
POST:
POST:Hit RETURN to continue
POST: s-lab f
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s x n 1e-28 1e-18
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 32b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: s-s y n 1e-4 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 32c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Finally plot how the composition of FCC varies.
POST: s-d-a y w(fcc_a1#1,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-s y n 1e-12 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 32d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex33

```
About
 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex33\tcex33.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Benchmark calculation for Fe-Cr-C isopleth
SYS: @@
SYS: set-log ex33,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw FEDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database

 VA                      /-  DEFINED
TDB_FEDEMO: d-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
   DEFINED
TDB_FEDEMO: rej ph /all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                BCC_A2
 CEMENTITE               CHI_A12                 DIAMOND_FCC_A4
 FCC_A1                  GRAPHITE                HCP_A3
 KSI_CARBIDE             LAVES_PHASE_C14         M23C6
 M3C2                    M5C2                    M7C3
 SIGMA   REJECTED
TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 graphite sigma cementite m23 m7 m3c2
   ... the command in full is RESTORE
 LIQUID:L                FCC_A1                  BCC_A2
 GRAPHITE                SIGMA                   CEMENTITE
 M23C6                   M7C3                    M3C2
   RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
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  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
TDB_FEDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1200,p=1e5,n=1 w(cr)=.13 w(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          9529 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 w(c) 0 .02
   ... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/: 5E-04
POLY_3: s-a-v 2 t 800 2000
   ... the command in full is SET_AXIS_VARIABLE
Increment /30/: 30
POLY_3: save tcex33 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
```

```
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.207E-03  8.100E+02
     BCC_A2
     M23C6
  ** M7C3
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.259E-03  8.000E+02
     BCC_A2
     M23C6
  ** M7C3
 Calculated.                     12  equilibria

 Phase region boundary   3 at:   3.778E-03  1.096E+03
     BCC_A2
  ** FCC_A1#2
     M23C6
  ** M7C3

 Phase region boundary   4 at:   3.778E-03  1.096E+03
     BCC_A2
  ** FCC_A1
     M23C6
 Calculated.                      9  equilibria

 Phase region boundary   5 at:   8.020E-05  1.125E+03
     BCC_A2
  ** FCC_A1
  ** M23C6

 Phase region boundary   6 at:   8.020E-05  1.125E+03
     BCC_A2
  ** FCC_A1
 Calculated                     16  equilibria

 Phase region boundary   7 at:   8.020E-05  1.125E+03
     BCC_A2
  ** M23C6
 Calculated..                     12  equilibria
 Terminating at axis limit.

 Phase region boundary   8 at:   8.020E-05  1.125E+03
     BCC_A2
     FCC_A1
  ** M23C6
 Calculated.                      4  equilibria

 Phase region boundary   9 at:   1.004E-03  1.155E+03
  ** BCC_A2
     FCC_A1
  ** M23C6

 Phase region boundary  10 at:   1.004E-03  1.155E+03
     FCC_A1
  ** M23C6
 Calculated.                      5  equilibria

 Phase region boundary  11 at:   2.216E-03  1.245E+03
     FCC_A1
  ** M23C6
  ** M7C3

 Phase region boundary  12 at:   2.216E-03  1.245E+03
     FCC_A1
  ** M23C6
     M7C3
 Calculated.                     10  equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   2.216E-03  1.245E+03
     FCC_A1
  ** M7C3
 Calculated.                     26  equilibria
```

```
Phase region boundary  14 at:    1.143E-02  1.569E+03
 ** LIQUID
    FCC_A1
 ** M7C3

Phase region boundary  15 at:    1.143E-02  1.569E+03
    LIQUID
    FCC_A1
 ** M7C3
Calculated..                     19  equilibria
Terminating at axis limit.

Phase region boundary  16 at:    1.143E-02  1.569E+03
 ** LIQUID
    FCC_A1
Calculated.                     17  equilibria

Phase region boundary  17 at:    4.634E-03  1.684E+03
 ** LIQUID
 ** BCC_A2
    FCC_A1

Phase region boundary  18 at:    4.634E-03  1.684E+03
 ** LIQUID
    BCC_A2
    FCC_A1
Calculated.                      8  equilibria

Phase region boundary  19 at:    1.464E-03  1.696E+03
 ** LIQUID
    BCC_A2
 ** FCC_A1

Phase region boundary  20 at:    1.464E-03  1.696E+03
 ** LIQUID
    BCC_A2
Calculated                     18  equilibria

Phase region boundary  21 at:    1.464E-03  1.696E+03
    BCC_A2
 ** FCC_A1
Calculated                     27  equilibria

Phase region boundary  22 at:    1.464E-03  1.696E+03
    LIQUID
    BCC_A2
 ** FCC_A1
Calculated.                     16  equilibria

Phase region boundary  23 at:    8.680E-03  1.714E+03
    LIQUID
 ** BCC_A2
 ** FCC_A1

Phase region boundary  24 at:    8.680E-03  1.714E+03
    LIQUID
 ** FCC_A1
Calculated..                     24  equilibria
Terminating at axis limit.

Phase region boundary  25 at:    8.680E-03  1.714E+03
    LIQUID
 ** BCC_A2
Calculated                     30  equilibria

Phase region boundary  26 at:    8.680E-03  1.714E+03
    LIQUID
 ** BCC_A2
    FCC_A1
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:    4.634E-03  1.684E+03
 ** BCC_A2
    FCC_A1
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:    1.143E-02  1.569E+03
 ** LIQUID
    FCC_A1
    M7C3
Calculated..                     19  equilibria
Terminating at axis limit.

Phase region boundary  29 at:    2.216E-03  1.245E+03
    FCC_A1
    M23C6
 ** M7C3
Calculated.                      7  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:    1.004E-03  1.155E+03
 ** BCC_A2
    FCC_A1
    M23C6
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:    4.772E-03  1.096E+03
    BCC_A2
 ** FCC_A1
    M7C3
Calculated..                     32  equilibria
Terminating at axis limit.

Phase region boundary  32 at:    5.640E-03  1.096E+03
 ** BCC_A2
    FCC_A1
    M7C3
Calculated..                     30  equilibria
Terminating at axis limit.

Phase region boundary  33 at:    4.772E-03  1.096E+03
    BCC_A2
 ** M23C6
```

```
    M7C3
Calculated..                     15  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  34 at:   7.207E-03  8.100E+02
    BCC_A2
    M23C6
 ** M7C3
Calculated.                     12  equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   5.000E-04  1.121E+03
    BCC_A2
 ** FCC_A1
    M23C6
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  36 at:   5.000E-04  1.121E+03
    BCC_A2
 ** FCC_A1
    M23C6
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   6.833E-03  8.723E+02
    BCC_A2
    M23C6
 ** M7C3
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  38 at:   6.833E-03  8.723E+02
    BCC_A2
    M23C6
 ** M7C3
Calculated..                      5  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  39 at:   1.317E-02  1.082E+03
    BCC_A2
 ** FCC_A1
    M7C3
Calculated.                     18  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   1.317E-02  1.082E+03
    BCC_A2
 ** FCC_A1
    M7C3
Calculated..                     15  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  41 at:   1.004E-02  8.100E+02
    BCC_A2
 ** M23C6
    M7C3
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  42 at:   1.004E-02  8.100E+02
    BCC_A2
 ** M23C6
    M7C3
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  43 at:   1.950E-02  1.061E+03
    BCC_A2
 ** FCC_A1
    M7C3
Calculated.                     31  equilibria
Terminating at known equilibrium

Phase region boundary  44 at:   1.950E-02  1.061E+03
    BCC_A2
 ** FCC_A1
    M7C3
Calculated..                      3  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  45 at:   7.664E-04  1.203E+03
 ** BCC_A2
    FCC_A1
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  46 at:   7.664E-04  1.203E+03
 ** BCC_A2
    FCC_A1
Calculated.                     18  equilibria
Terminating at known equilibrium

Phase region boundary  47 at:   3.363E-03  1.203E+03
    FCC_A1
 ** M23C6
    M7C3
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  48 at:   3.363E-03  1.203E+03
    FCC_A1
 ** M23C6
    M7C3
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  49 at:   7.811E-04  1.597E+03
    BCC_A2
 ** FCC_A1
Calculated                     27  equilibria
```

```
 Phase region boundary  50 at:   7.811E-04  1.597E+03
     BCC_A2
  ** FCC_A1
 Calculated.                      5  equilibria
 Terminating at known equilibrium

 Phase region boundary  51 at:   9.892E-03  1.597E+03
  ** LIQUID
     FCC_A1
 Calculated.                      5  equilibria
 Terminating at known equilibrium

 Phase region boundary  52 at:   9.892E-03  1.597E+03
  ** LIQUID
     FCC_A1
 Calculated.                     14  equilibria
 Terminating at known equilibrium

 Phase region boundary  53 at:   5.000E-04  1.788E+03
     LIQUID
  ** BCC_A2
 Calculated                     22  equilibria

 Phase region boundary  54 at:   5.000E-04  1.788E+03
     LIQUID
  ** BCC_A2
 Calculated.                     18  equilibria
 Terminating at known equilibrium

 Phase region boundary  55 at:   6.833E-03  1.730E+03
     LIQUID
  ** BCC_A2
 Calculated                     26  equilibria

 Phase region boundary  56 at:   6.833E-03  1.730E+03
     LIQUID
  ** BCC_A2
 Calculated.                      5  equilibria
 Terminating at known equilibrium

 Phase region boundary  57 at:   1.317E-02  1.691E+03
     LIQUID
  ** FCC_A1
 Calculated.                     10  equilibria
 Terminating at known equilibrium

 Phase region boundary  58 at:   1.317E-02  1.691E+03
     LIQUID
  ** FCC_A1
 Calculated..                     15  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

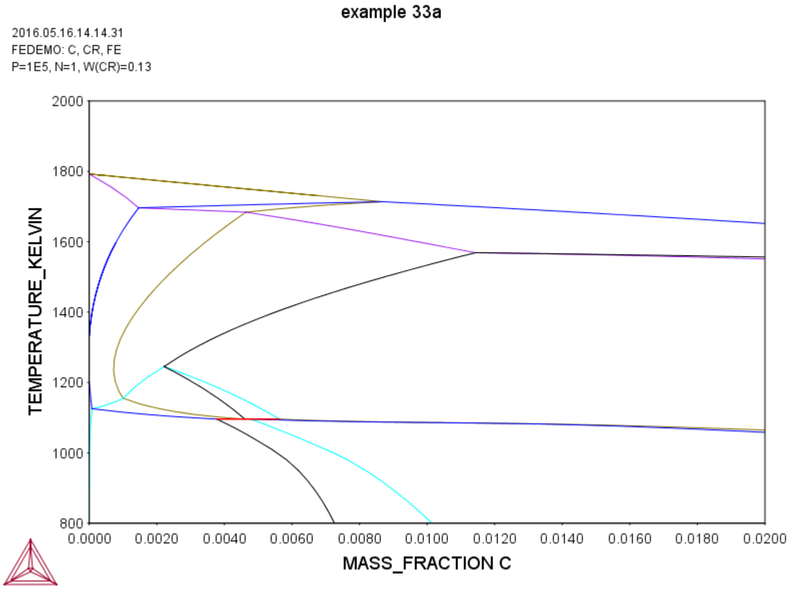
 Phase region boundary  59 at:   1.950E-02  1.655E+03
     LIQUID
  ** FCC_A1
 Calculated.                     23  equilibria
 Terminating at known equilibrium

 Phase region boundary  60 at:   1.950E-02  1.655E+03
     LIQUID
  ** FCC_A1
 Calculated..                      3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex33\tcex
 33.POLY3
 CPU time for mapping                        5  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST: set-title example 33a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
```

```
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex34

```
About
 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\tcex34.TCM"SYS: set-echo
SYS: @@
SYS: @@ Calculation
SYS: @@ of the phase diagram and G curves
SYS: @@ in the Al-Zn system
SYS: @@
SYS: @@ Another example of using the BINARY module
SYS: @@
SYS: go bin
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase_Diagram
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES5 .....
 AL                      ZN  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  TETRAGONAL_A6           RHOMBOHEDRAL_A7
 CBCC_A12                CUB_A13                 B32_ALLI
 B3_ZINCBLENDE           C14_LAVES               C15_LAVES
 C16_AL2CU               C36_LAVES               D019_AL1M3
 D513_AL3NI2             D82_FEZN_GAMMA          L10_ALTI
 AGZN_ZETA               AL5FE4                  ALCE_AMORPHOUS
 ALCU_ETA                FEZN4                   FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 HCP_ZN  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
 -OK-
 The condition X(ZN)=.1234  created
 The condition T=612.43  created
 Forcing automatic start values
 Automatic start values will be set
 Start points provided by database
 Version S mapping is selected

 Organizing start points

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   5.345E-01  5.000E+02
  ** FCC_A1
     HCP_ZN
 Calculated..                      10  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   5.027E-01  3.000E+02
  ** FCC_A1
     HCP_ZN
 Calculated.                      13  equilibria

 Phase region boundary   3 at:   5.626E-01  5.504E+02
  ** FCC_A1
  ** FCC_A1#2
     HCP_ZN

 Phase region boundary   4 at:   7.872E-01  5.504E+02
  ** FCC_A1
     HCP_ZN
 Calculated.                       6  equilibria

 Phase region boundary   5 at:   8.211E-01  6.540E+02
  ** LIQUID
  ** FCC_A1
     HCP_ZN

 Phase region boundary   6 at:   9.263E-01  6.540E+02
  ** LIQUID
     HCP_ZN
```

```
Calculated                       17  equilibria

Phase region boundary   7 at:   7.783E-01  6.540E+02
 ** LIQUID
    FCC_A1
Calculated                       73  equilibria

Phase region boundary   8 at:   3.658E-01  5.504E+02
 ** FCC_A1
    FCC_A1#2
Calculated                       27  equilibria

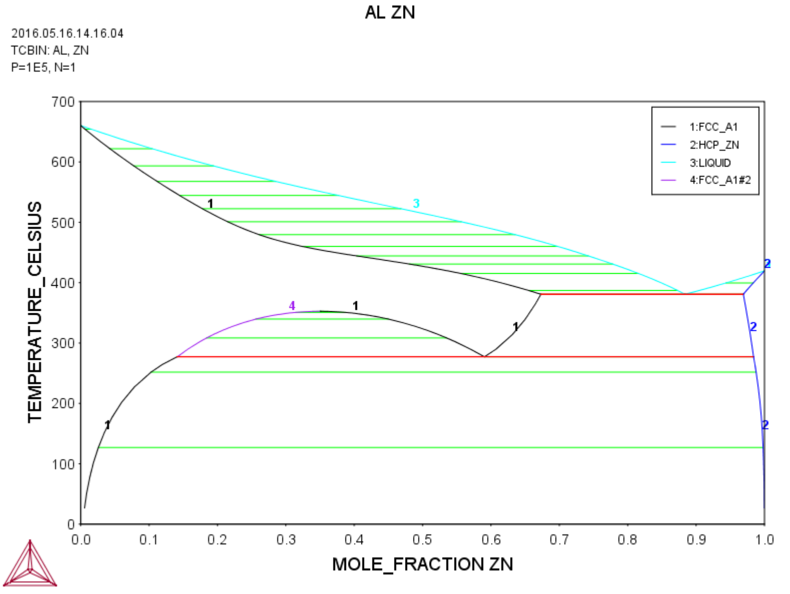
Phase region boundary   9 at:   5.345E-01  5.000E+02
 ** FCC_A1
    HCP_ZN
Calculated.                        5  equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\BINA
RY.POLY3
CPU time for mapping                         1  seconds

 POSTPROCESSOR VERSION 3.2

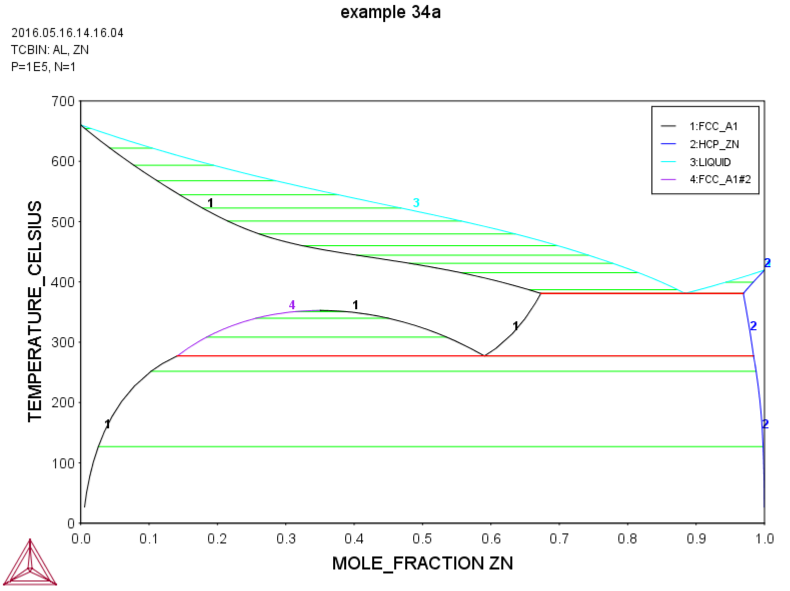

Setting automatic diagram axes


 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes
```



```
POST: set-title example 34a
POST: plot
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot a G curve at 573 K!
POST: back
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                  B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
SYS: go bin
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                  B2_VACANCY
```

```
 HIGH_SIGMA               DICTRA_FCC_A1   REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC Binary Solutions  v1.1

 VA                       /-   DEFINED
 BCC_B2                   FCC_L12                  FCC_L102
 D021_HCP  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G
Temperature (C): /1000/: 300
 VA                       /-   DEFINED
 BCC_B2                   FCC_L12                  FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES5 .....
 AL                       ZN  DEFINED
 GAS:G                    LIQUID:L                 IONIC_LIQUID:Y
 FCC_A1                   BCC_A2                   A2_BCC
 HCP_A3                   HCP_ZN                   DIAMOND_A4
 BCT_A5                   TETRAGONAL_A6            RHOMBOHEDRAL_A7
 CBCC_A12                 CUB_A13                  B32_ALLI
 B3_ZINCBLENDE            C14_LAVES                C15_LAVES
 C16_AL2CU                C36_LAVES                D019_AL1M3
 D513_AL3NI2              D82_FEZN_GAMMA           L10_ALTI
 AGZN_ZETA                AL5FE4                   ALCE_AMORPHOUS
 ALCU_ETA                 FEZN4                    FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 HCP_ZN  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

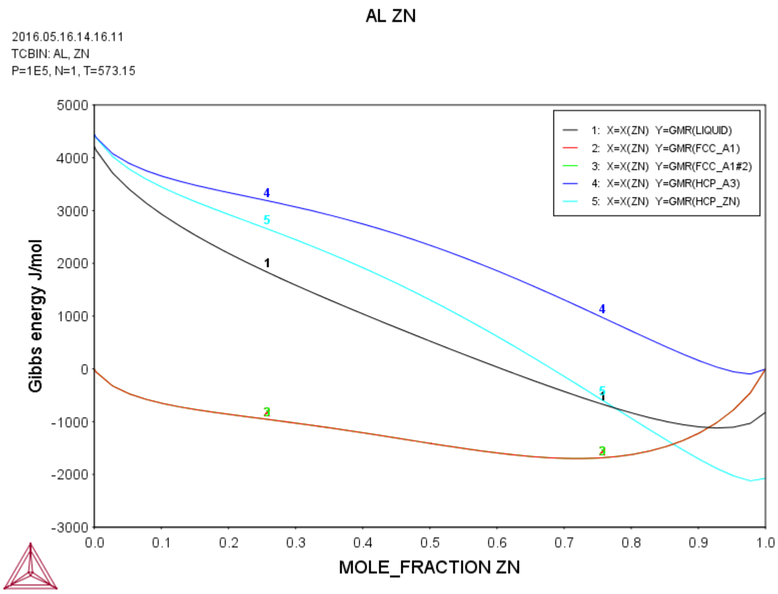
 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
 -OK-
 The condition X(ZN)=.1234  created
 Forcing automatic start values
 Automatic start values will be set

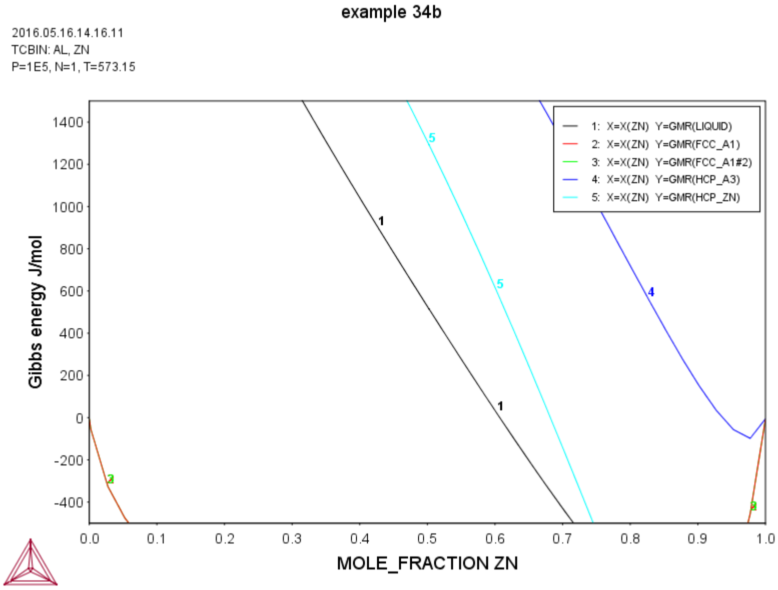
 Phase Region from   0.502463     for:
     LIQUID
     FCC_A1
     FCC_A1#2
     HCP_A3
     HCP_ZN

 Phase Region from   0.502463     for:
     LIQUID
     FCC_A1
     FCC_A1#2
     HCP_A3
     HCP_ZN
 *** Buffer saved on file ***
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\GCUR
 VE.POLY3

  POSTPROCESSOR VERSION 3.2
```



```
POST: s-s y n -500 1500
POST:
POST: set-title example 34b
POST:
POST: plot
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot an activity (A) curve at 573 K
POST: back
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
SYS: go bin
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: A
Temperature (C): /1000/: 300
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES5 .....
 AL                      ZN  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  TETRAGONAL_A6           RHOMBOHEDRAL_A7
 CBCC_A12                CUB_A13                 B32_ALLI
 B3_ZINCBLENDE           C14_LAVES               C15_LAVES
 C16_AL2CU               C36_LAVES               D019_AL1M3
 D513_AL3NI2             D82_FEZN_GAMMA          L10_ALTI
 AGZN_ZETA               AL5FE4                  ALCE_AMORPHOUS
 ALCU_ETA                FEZN4                   FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 HCP_ZN  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
 -OK-
 The condition X(ZN)=.1234  created

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Forcing automatic start values
 Automatic start values will be set
 No initial equilibrium, using default
 Step will start from axis value   0.123400
...OK

 Phase Region from   0.123400      for:
     FCC_A1
 Global test at  3.23400E-01 .. Backtracking to find phase change for FCC_A1#2
 Global test at  1.48400E-01 .... OK
 Global check of adding phase at  1.70853E-01
 Calculated      5 equilibria

 Phase Region from   0.170853      for:
     FCC_A1
     FCC_A1#2
 Global test at  3.48400E-01 .... OK
```

```
 Global check of removing phase at  5.51861E-01
 Calculated    19 equilibria

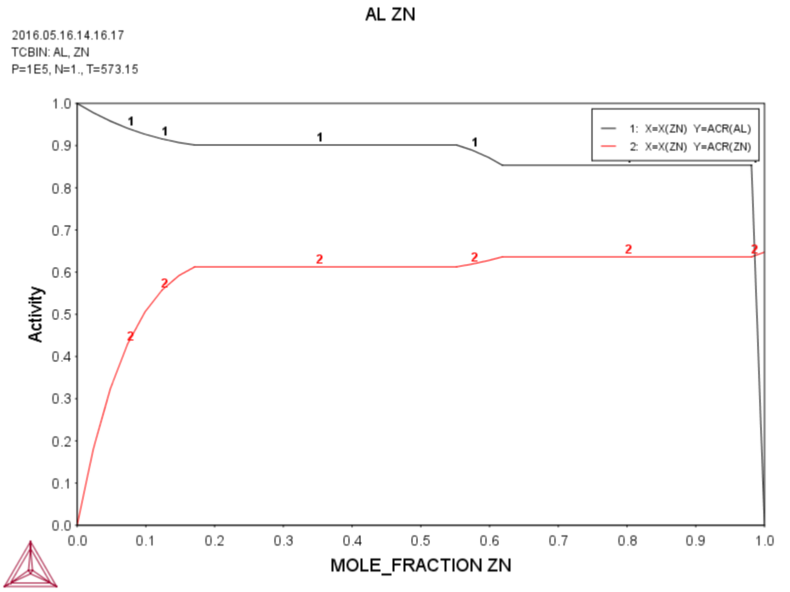
 Phase Region from   0.551861      for:
     FCC_A1#2
 Global check of adding phase at  6.18456E-01
 Calculated     5 equilibria

 Phase Region from   0.618456      for:
     FCC_A1#2
     HCP_ZN
 Global test at  7.98400E-01 .... OK
 Global check of removing phase at  9.81102E-01
 Calculated    18 equilibria

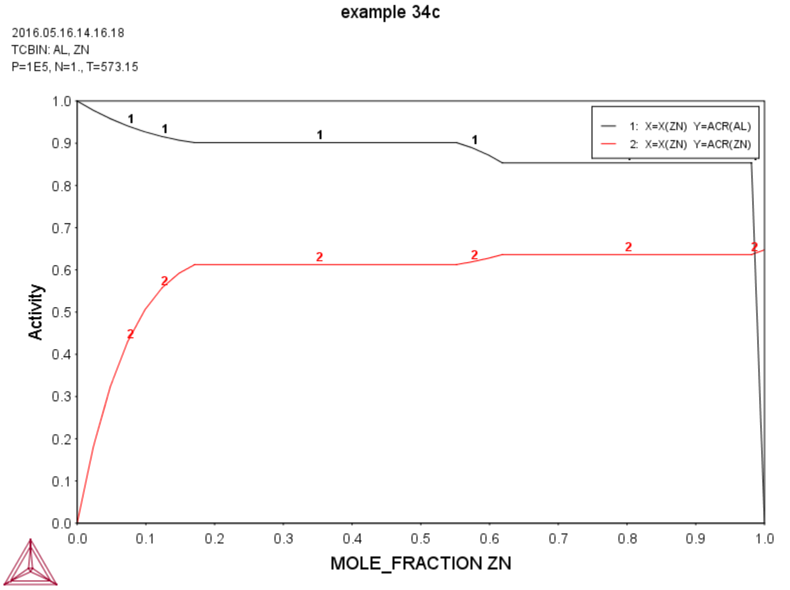
 Phase Region from   0.981102      for:
     HCP_ZN
 Terminating at    1.00000
 Calculated     4 equilibria

 Phase Region from   0.123400      for:
     FCC_A1
 Terminating at   0.100000E-11
 Calculated     8 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\GCUR
 VE.POLY3

  POSTPROCESSOR VERSION 3.2
```



```
POST:
POST: set-title example 34c
POST:
POST: plot
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot a Phase fraction (F) curve for x(zn)=.5.
POST: @@ The miscibility gap can be found now
POST: back
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
SYS: go bin
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
```

```
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: F
Fraction of: zn /.5/: .5
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES5 .....
 AL                      ZN  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  TETRAGONAL_A6           RHOMBOHEDRAL_A7
 CBCC_A12                CUB_A13                 B32_ALLI
 B3_ZINCBLENDE           C14_LAVES               C15_LAVES
 C16_AL2CU               C36_LAVES               D019_AL1M3
 D513_AL3NI2             D82_FEZN_GAMMA          L10_ALTI
 AGZN_ZETA               AL5FE4                  ALCE_AMORPHOUS
 ALCU_ETA                FEZN4                   FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 HCP_ZN  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
 -OK-
 Forcing automatic start values
 Automatic start values will be set
 No initial equilibrium, using default
 Step will start from axis value   1000.000
...OK

 Phase Region from   1000.000     for:
     LIQUID
 Global test at  9.20000E+02 .... OK
 Global test at  8.20000E+02 .... OK
 Global check of adding phase at  7.88048E+02
 Calculated    24 equilibria

 Phase Region from    788.048     for:
     LIQUID
     FCC_A1
 Global test at  7.26000E+02 .... OK
 Global test at  7.06000E+02 .... OK
 Global check of removing phase at  7.00299E+02
 Calculated    23 equilibria

 Phase Region from    700.299     for:
     FCC_A1
 Global test at  6.28000E+02 .... OK
 Global test at  5.28000E+02 .. Backtracking to find phase change for FCC_A1#2
 Global test at  6.18000E+02 .... OK
 Global test at  5.98000E+02 .... OK
 Global check of adding phase at  5.96831E+02
 Calculated    15 equilibria

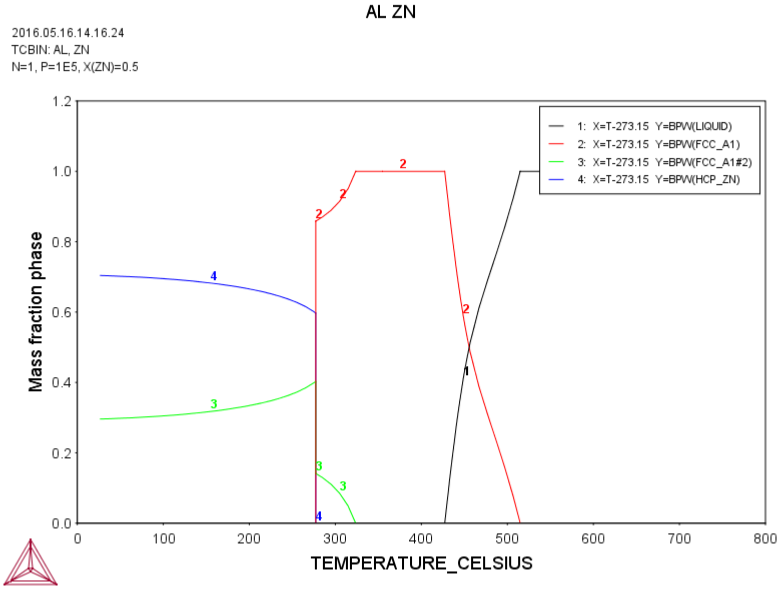
 Phase Region from    596.831     for:
     FCC_A1
     FCC_A1#2
 Global check of adding phase at  5.50386E+02
 Calculated     7 equilibria

 Phase Region from    550.386     for:
     FCC_A1
     FCC_A1#2
     HCP_ZN
 Calculated     2 equilibria

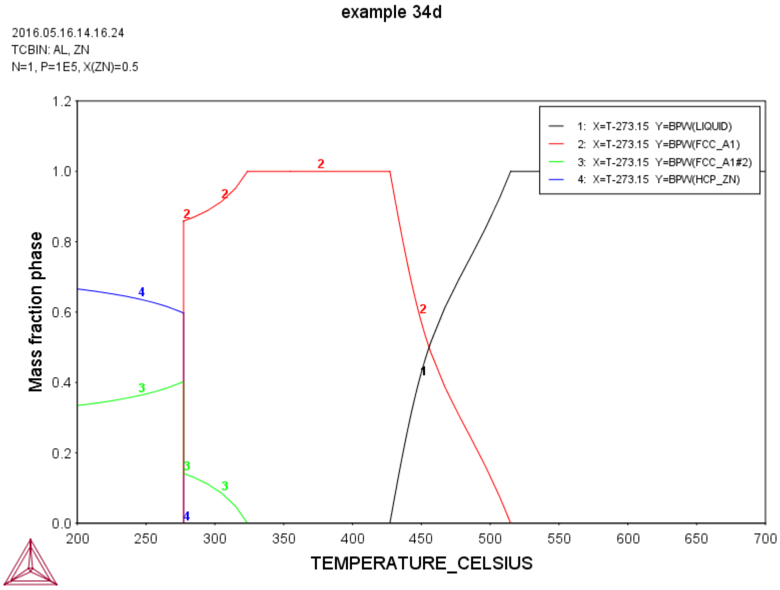
 Phase Region from    550.386     for:
     FCC_A1#2
     HCP_ZN
 Global test at  4.78000E+02 .... OK
 Global test at  3.78000E+02 .... OK
 Terminating at    300.000
 Calculated    29 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\PFCU
 RVE.POLY3

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes
```



```
POST:
POST: s-s x n 200 700
POST: set-title example 34d
POST:
POST: plot
```



```
POST:
POST: set-inter
POST:
```

tcex35

```
About Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex35\tcex35.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example of use of the POTENTIAL module
SYS: @@
SYS: go pot

 Simple potential phase diagram calculation module

Database: /POT/: SUBDEMO
 THERMODYNAMIC DATABASE module
 Current database: Substance Demo Database

 VA                       /-  DEFINED
Matrix element: /FE/: FE
First potential species: /S1O2/: C1O1
Second potential species: /O2/: O2
Temperature: /1000/: 1000
 VA                       /-  DEFINED
 REINITIATING GES5 .....
 FE                       C                        O
   DEFINED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'C1<G> T.C.R.A.S. Class: 1 C1<G> C<G>'
  'C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE ** C1O1<G> CO<G> CARBON MONOXIDE
      <GAS> STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65'
  'C1O2<G> T.C.R.A.S. Class: 2 C1O2<G> CO2<G> CARBON DIOXIDE <GAS>'
  'C2<G> T.C.R.A.S. Class: 2 C2<G> CARBON Diatomic Gas.'
  'C2O1<G> T.C.R.A.S. Class: 5 C2O1<G> C2O<G>'
  'C3<G> T.C.R.A.S. Class: 6 C3<G> CARBON <TRIATOMIC GAS>'
  'C3O2<G> T.C.R.A.S. Class: 6 C3O2<G>'
  'C4<G> T.C.R.A.S. Class: 7 C4<G>'
  'C5<G> T.C.R.A.S. Class: 7 C5<G>'
  'C5FE1O5<G> JANAF 1982 SGTE C5FE1O5<G> Fe(CO)5<G> IRON PENTACARBONYL <GAS>
      ASSESSMENT DATED 3/78'
  'C60<G> MHR-95 C60<G> Data processed from [94Kor/Sid] M.V. Korobov, L.N.
      sidorov, J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the
      rotational data in [91McK] and vibration frequencies in [94Kor/Sid].
      Note that a frequency with degeneracy 5 is missing from list in
      [94Kor/Sid]; taken to be 419 cm-1, which gives very good, though not
      exact, agreement with values quoted in [94Kor/Sid]. Note discrepancy
      between calculated DrS(298) = -8943.5 J mol K-1 for the reaction 60C<g>
      =C60<g>and that given by [94Kor/Sid] in their Table 5, -8950 J mol K
      -1. Enthalpy of formation: DfH = 2588 kJ/mol from DsubH(298.15K) = 166
      +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure values reproduced very
      well. [91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).'
  'FE1<G> THERMODATA FE1<G> Fe<G> Data provided by T.C.R.A.S. October 1996
      Modified by Thermodata - new assessment'
  'FE1O1<G> TCRAS 5-F FEO IRON OXIDE 23/11/06 FE1O1<G> FeO<G>'
  'FE1O2<G> T.C.R.A.S Class: 6 FE1O2<G> FeO2<G> Data provided by TCRAS.
      October 1996. Error in version 1997. S298 corrected to 1bar 20080222
      AAZ TCRAS2006 : dH, S'
  'FE2<G> THERMODATA FE2<G> Fe2<G> Data provided by T.C.R.A.S. October 1996
      Modified by Thermodata - new assessment. Typing error corrected 12/06'
  'O2<G> TCRAS 21/06/90 O2<G> OXYGEN Gaseous Standard State.'
  'O3<G> TCRAS 02/06/80 O3<G> OZONE Gaseous Standard State.'
  'C1FE1O3 N.P.L. SGTE ** C1FE1O3 FeCO3 Siderite IRON<2> CARBONATE
      DECOMPOSES BEFORE FUSION.'
  'C1FE3 N.P.L. SGTE ** C1FE3 Fe3C Cementite CEMENTITE'
  'C5FE1O5<L> I. BARIN 3rd. Edition C5FE1O5_Liquid Fe(CO)5_Liquid IRON
      PENTACARBONYL (Liquid). Same as in previous versions. Rounding of H298.'
  'C60 MHR-95 C60 Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
       J. Chem. The Fitted to the data in [94Kor/Sid], who took the phase
      transition at 257K that [94Kor/Sid] do not give an explicit value for
      S(298.15K). S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =
      425.8 and Cp e calculated from DrS(298) for 60C<graphite>=C60 given by
      [94Kor/Sid] in their Table 5, which gives S(298.15K) = 425.4 J mol K
      -1. Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
       the value preferred, if obliquely, by [94Kor/Sid]. [92Ste/Chi]W.V.
      Steele, R.D. Chirico, N.K. Smith, W.e. Billups, P.R. Elmore, A.E.
      Wheeler, J. Phys. Chem. 96 4731 (1993).'
  'C1<DIAMOND> S.G.T.E. ** C_DIAMOND <DIAMOND> Data from SGTE Unary DB, data
      added by atd 7/9/95, H298-H0 taken from 1994 database (ex THERMODATA
      01/93)'
  'FE1O1 T.C.R.A.S Class: 5 FE1O1 FeO FeO_Wustite IRON OXIDE. Data provided
      by T.C.R.A.S. in 2000'
  'FE2O3<FE2O3_GAMMA> T.C.R.A.S Class: 5 FE2O3_GAMMA Fe2O3_Gamma Data
      provided by T.C.R.A.S. in 2000'
  'FE1 S.G.T.E. ** FE1 Fe Data from SGTE Unary DB'
  'C1<GRAPHITE> S.G.T.E. ** C_GRAPHITE Data from SGTE Unary DB, pressure
      dependent data added by atd 7/9/95'
  'FE2O3<HEMATITE> T.C.R.A.S Class: 7 FE2O3 Fe2O3 Hematite Data provided by
      T.C.R.A.S. in 2000 with previous description of the magnetic
      transition fitted by IA. In version 2000 only H298 has been changed.'
  'FE3O4<MAGNETITE> JANAF 4th Ed. FE3O4 Fe3O4 MAGNETITE Data refitted by IA
      to reproduce the magnetic transition.'
  'FE0.947O1<WUSTITE> T.C.R.A.S Class: 5 FE0.947O1 Fe0.947O WUSTITE WUSTITE.
      Data provided by T.C.R.A.S. in 2000 20080222 AAZ TCRAS2006 : dH, S'
 -OK-
 This command is DEPRECATED and to be removed in the future!

 Please use ADVANCED_OPTIONS instead of SPECIAL_OPTIONS

 The condition LNACR(C1O1,GAS)=-140.8589  created
 The condition LNACR(O2,GAS)=-140.8589  created
 Normal POLY minimization, not global
 Version S mapping is selected

 Organizing start points
```

```
Using ADDED start equilibria

 Working hard
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4

 Phase region boundary   1 at:  -4.633E+01 -1.409E+02
     FE_S
  ** GRAPHITE
 Calculated..                     81  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:  -1.259E+02 -3.000E+02
     FE_S
  ** GRAPHITE
 Calculated.                    126  equilibria

 Phase region boundary   3 at:  -9.383E-01 -5.007E+01
  ** FE1O1_S
     FE_S
  ** GRAPHITE

 Phase region boundary   4 at:  -9.383E-01 -5.007E+01
  ** FE1O1_S
     FE_S
 Calculated..                    151  equilibria
 Terminating at axis limit.

 Phase region boundary   5 at:  -9.383E-01 -5.007E+01
  ** FE1O1_S
     GRAPHITE
 Calculated.                      2  equilibria

 Phase region boundary   6 at:  -3.398E-01 -4.887E+01
  ** GAS
  ** FE1O1_S
     GRAPHITE

 Phase region boundary   7 at:  -3.398E-01 -4.887E+01
  ** GAS
     GRAPHITE

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 Phase region boundary   8 at:  -3.398E-01 -4.887E+01
  ** GAS
     FE1O1_S
 Calculated.                      7  equilibria

 Phase region boundary   9 at:  -3.272E+00 -4.059E+01
  ** GAS
     FE1O1_S
  ** MAGNETITE

 Phase region boundary  10 at:  -3.272E+00 -4.059E+01
     FE1O1_S
  ** MAGNETITE
 Calculated..                    150  equilibria
 Terminating at axis limit.

 Phase region boundary  11 at:  -3.272E+00 -4.059E+01
     GAS
  ** MAGNETITE
 Calculated.                     10  equilibria

 Phase region boundary  12 at:  -1.174E+01 -2.359E+01
     GAS
  ** HEMATITE
  ** MAGNETITE

 Phase region boundary  13 at:  -1.174E+01 -2.359E+01
     GAS
  ** HEMATITE
 Calculated..                    168  equilibria
 Terminating at axis limit.

 Phase region boundary  14 at:  -1.174E+01 -2.359E+01
  ** HEMATITE
     MAGNETITE
 Calculated..                    146  equilibria
 Terminating at axis limit.

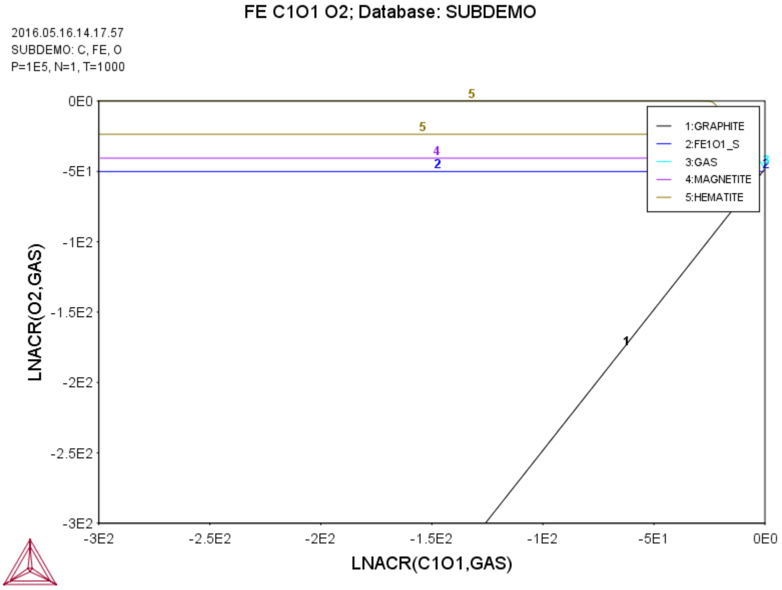
 Phase region boundary  15 at:  -4.633E+01 -1.409E+02
     FE_S
  ** GRAPHITE
 Calculated.                     47  equilibria
 Terminating at known equilibrium

 Phase region boundary  16 at:  -1.409E+02 -5.007E+01
  ** FE1O1_S
     FE_S
 Calculated..                     81  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

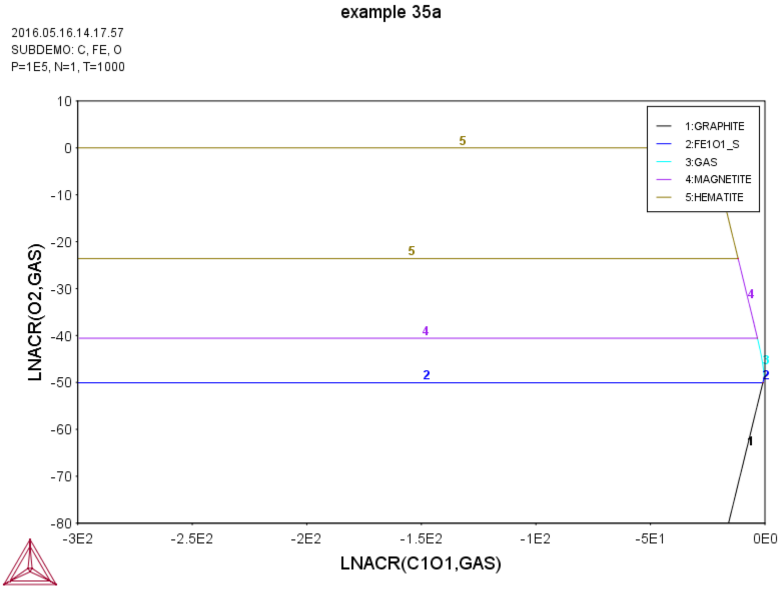
 Phase region boundary  17 at:  -1.409E+02 -5.007E+01
  ** FE1O1_S
     FE_S
 Calculated.                     71  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex35\POT.
 POLY3
 CPU time for mapping                      1  seconds

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes
```



```
POST: s-s y n -80 10
POST: set-title example 35a
POST:
POST: pl
```



```
POST:
POST: set-inter
POST:
```

tcex36a

```
SYS:AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tcex36a.TCM"SYS: set-echo
SYS: @@
SYS: @@ Assessment. The use of the PARROT module
SYS: @@
SYS: @@ This is the setup file for windows systems
SYS: @@
SYS: set_log tcex36a,,,,
SYS: @@ First the elements and phases must be entered in G-E-S module
SYS: GO G
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: ENTER-ELEMENT A B
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
GES: AMEND-ELEMENT-DATA A BCC 20 0 0 1
GES: AMEND-ELEMENT-DATA B BCC 50 0 0 1
GES: ENTER-PHASE LIQUID L 1 A B; N N
GES: ENTER-PHASE BCC,, 1 A B; N N
GES: ENTER-PHASE FCC,, 1 A B; N N
GES: ENTER-PHASE A2B,, 2 2 1 A; B; N N
 CONSTITUENTS IN SUBLATTICE                      1
 CONSTITUENTS IN SUBLATTICE                      2
GES: @@ There is a miscibility gap in the bcc, this must be stated here
GES: AMEND_PHASE BCC COMPOSITION_SETS 2 B
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES: @@ We can also set the major constituent of the first composition set
GES: AMEND_PHASE BCC MAJOR 1 A
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: @@ The FCC phase is stable only for element B
GES: AMEND_PHASE FCC MAJOR 1 B
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES: @@ the parameters can be entered in the PARROT module
GES: GO PAR
   ... the command in full is GOTO_MODULE

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: ENTER-PARAMETER G(BCC,A) 500 0; 2000 N
 G(BCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(BCC,B) 500 0; 2000 N
 G(BCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A) 500 14000-10*T; 2000 N
 G(LIQUID,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(LIQUID,B) 500 18000-12*T; 2000 N
 G(LIQUID,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,B) 500 3300-3*T; 2000 N
 G(FCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,A) 500 408; 2000 N
 G(FCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(A2B) 500 V1+V2*T+V3*T*LOG(T); 2000 N
 G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;0) 500 V11+V12*T; 2000 N
 G(LIQUID,A,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;1) 500 V13+V14*T; 2000 N
 G(LIQUID,A,B;1)
PARROT: ENTER-PARAMETER G(BCC,A,B;0) 500 V15+V16*T; 2000 N
 G(BCC,A,B;0)
PARROT: ENTER-PARAMETER G(BCC,A,B;1) 500 V17+V18*T; 2000 N
 G(BCC,A,B;1)
PARROT: ENTER-PARAMETER G(FCC,A,B;0) 500 V19+V20*T; 2000 N
 G(FCC,A,B;0)
PARROT: ENTER-PARAMETER G(FCC,A,B;1) 500 V21+V22*T; 2000 N
 G(FCC,A,B;1)
PARROT:
PARROT: @@ everything is saved on an unformatted work file by the create command
PARROT: CREATE tcex36
   ... the command in full is CREATE_NEW_STORE_FILE
PARROT:
PARROT:Hit RETURN to continue
PARROT:
PARROT: @@ the experimental data file is compiled to the work file.
PARROT: COMPILE tcex36 screen Y exp36
   ... the command in full is COMPILE_EXPERIMENTS
A new feature is that POP files may include graphics information using the
GRAPHICS_PLOT command. A file name for generating an ".exp" file must be given.
 $
 $ POP file for assessment example
 $
 $ Enter some constants used later.
 ENTER_SYMBOL CONSTANT  DX=0.02,P0=101325,DH=500,DT=10
 $
 $ Eutectic point at A rich side from ref #2.
 $ T=1193 K, 40.8 w/o B in liquid, 13 w/o B in bcc.
 $ In a binary system one must have four conditions if P is not fixed.
 $ We obtain this by fixing the pressure and that three phases must be stable.
 $ The amount of the fixed phases is irrelevant here
 CREATE_NEW_EQUILIBRIUM 1,1
 CHANGE_STATUS PHASE LIQUID,BCC,A2B=FIX 1
 SET-CONDITION P=P0
 EXPERIMENT  T=1193:DT,W(LIQ,B)=.408:DX,W(BCC,B)=.13:DX
 GRAPHICS 1 .408 1193 MS5
   ... the command in full is GRAPHICS_PLOT
 GRAPHICS 1 .13  1193 DS5
   ... the command in full is GRAPHICS_PLOT
 GRAPHICS 1 .555 1193 DS5
   ... the command in full is GRAPHICS_PLOT
 LABEL AINV
   ... the command in full is LABEL_DATA
 SET-ALT X(A2B,A)=.6666667
   ... the command in full is SET_ALTERNATE_CONDITION
 SET_ALL_START  1193 Y
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
 $
```

```
$ Congrent melting temperature for A2B 1341 K.
$ We will include the enthalpy of transformation also and this
$ requires a function.
ENTER_SYMBOL FUNCTION  HTR=HM(LIQUID)-HM(A2B);
$
$ Note how one specifies that this is a congruent transformation!
CREATE_NEW_EQUILIBRIUM 2,1
CHANGE_STATUS PHASE LIQ,A2B=FIX 1
SET-CONDITION P=P0,X(LIQ,B)-X(A2B,B)=0
EXPERIMENT  T=1341:DT
EXPERIMENT  HTR=3727:500
GRAPHICS 1 .555 1341 MS7
  ... the command in full is GRAPHICS_PLOT
LABEL AINV
  ... the command in full is LABEL_DATA
SET-ALT X(A)=.6666667
  ... the command in full is SET_ALTERNATE_CONDITION
SET_ALL_START  1341 Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ Eutectic point at B rich side.
$ T=1049 K, 27 w/o A in liquid, 9.3 w/o A in bcc.
CREATE_NEW_EQUILIBRIUM 3,1
CHANGE_STATUS PHASE LIQ,BCC,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT  T=1049:DT,W(LIQ,A)=.27:DX,W(BCC,A)=.093:DX
SET-ALT X(A2B,A)=.66666667
  ... the command in full is SET_ALTERNATE_CONDITION
GRAPHICS 1 .907 1049 MS5
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .73  1049 DS5
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .555 1049 DS5
  ... the command in full is GRAPHICS_PLOT
LABEL AINV
  ... the command in full is LABEL_DATA
SET_ALL_START  1049 Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ Peritectic point. T=1203 K, 19 w/o A in liquid, 6.9 w/o A in bcc,
$ 6.0 w/o A in fcc.
CREATE_NEW_EQUILIBRIUM 4,1
CHANGE_STATUS PHASE LIQ,BCC,FCC=FIX 1
SET-CONDITION P=P0
EXPERIMENT  T=1203:DT,W(LIQ,A)=.19:DX,W(BCC,A)=.069:DX,W(FCC,A)=.06:DX
GRAPHICS 1 .81 1203 MS5
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .931 1203 DS5
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .94 1203 DS5
  ... the command in full is GRAPHICS_PLOT
LABEL AINV
  ... the command in full is LABEL_DATA
SET_ALL_START  1203 Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ Eutectoid transformation of A2B -> BCC1 + BCC2, from ref #3
$ T=726, 3.7 at/o B in A, 11.4 at/o A in B
$ Note that miscibility gaps are indicated by using # after the phase
$ name and then give an integer.
CREATE_NEW_EQUILIBRIUM 5,1
CHANGE_STATUS PHASE BCC#1,BCC#2,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT  T=726:DT,X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
SET-ALT X(A2B,A)=.6666667
  ... the command in full is SET_ALTERNATE_CONDITION
GRAPHICS 1 0.09 726 MS5
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 0.95 726 DS5
  ... the command in full is GRAPHICS_PLOT
LABEL AINV
  ... the command in full is LABEL_DATA
SET_ALL_START  726 Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ It is sometimes useful to decribe an invariant equilibria as
$ three tie-lines between each pair of phases at the same temperature.
$ In this case it helps to add a tie-line across the miscibility gap
$ at the invariant temperature.
CREATE_NEW_EQUILIBRIUM 6,1
CHANGE_STATUS PHASE BCC#1,BCC#2=FIX 1
SET-CONDITION P=P0 T=726
EXPERIMENT  X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
LABEL AINV
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ From ref #4 the liquidus at the B rich end:
$ The table values are referenced inside the table_head using @<column>
TABLE_HEAD 10
CREATE_NEW_EQUILIBRIUM 0010,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1594,P=P0
EXPERIMENT  W(LIQ,A)=0.02:DX
LABEL ALF
  ... the command in full is LABEL_DATA
GRAPHICS 1 .98 1594 MS5
  ... the command in full is GRAPHICS_PLOT
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0011,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1548,P=P0
EXPERIMENT  W(LIQ,A)=0.042:DX
LABEL ALF
  ... the command in full is LABEL_DATA
GRAPHICS 1 .958 1548 MS5
  ... the command in full is GRAPHICS_PLOT
SET_ALL_START Y
```

```
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0012,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1499,P=P0
EXPERIMENT  W(LIQ,A)=0.065:DX
LABEL ALF
  ... the command in full is LABEL_DATA
GRAPHICS 1 .935 1499 MS5
  ... the command in full is GRAPHICS_PLOT
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0013,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1438,P=P0
EXPERIMENT  W(LIQ,A)=0.093:DX
LABEL ALF
  ... the command in full is LABEL_DATA
GRAPHICS 1 .907 1438 MS5
  ... the command in full is GRAPHICS_PLOT
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set

$
$ From ref #5 we have the following tie-lines
TABLE_HEAD 20
CREATE_NEW_EQUILIBRIUM 0020,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1413,P=P0
EXPERIMENT  W(LIQ,A)=.104:DX,W(FCC,A)=.038:DX
GRAPHICS 1 .896 1413 MS9
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .962 1413 DS9
  ... the command in full is GRAPHICS_PLOT
LABEL ATIE
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
SET_START_VALUE  Y(LIQ,A)=.104,Y(FCC,A)=.038
CREATE_NEW_EQUILIBRIUM 0021,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1337,P=P0
EXPERIMENT  W(LIQ,A)=.136:DX,W(FCC,A)=.047:DX
GRAPHICS 1 .864 1337 MS9
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .953 1337 DS9
  ... the command in full is GRAPHICS_PLOT
LABEL ATIE
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
SET_START_VALUE  Y(LIQ,A)=.136,Y(FCC,A)=.047
CREATE_NEW_EQUILIBRIUM 0022,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1213,P=P0
EXPERIMENT  W(LIQ,A)=.187:DX,W(FCC,A)=.059:DX
GRAPHICS 1 .813 1213 MS9
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .941 1213 DS9
  ... the command in full is GRAPHICS_PLOT
LABEL ATIE
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
SET_START_VALUE  Y(LIQ,A)=.187,Y(FCC,A)=.059
CREATE_NEW_EQUILIBRIUM 0023,1
CHANGE_STATUS PHASE LIQ,BCC=FIX 1
SET-CONDITION T=1100,P=P0
EXPERIMENT  W(LIQ,A)=.245:DX,W(BCC,A)=.085:DX
GRAPHICS 1 .755 1100 MS9
  ... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .915 1100 DS9
  ... the command in full is GRAPHICS_PLOT
LABEL ATIE
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
SET_START_VALUE  Y(LIQ,A)=.245,Y(BCC,A)=.085

$
$ Thermochemical data
$ Activities of B in liquid (reference state fcc) at 1573 K.
$ The command SET_REFERENCE_STATE is used for this as the default
$ reference state for B is BCC.
$
$ Note that we have set an uncertainity on the fraction (condition) also.
TABLE_HEAD 100
CREATE_NEW_EQUILIBRIUM 0100,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.90:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.94:DX
GRAPHICS 3 .90 .94 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0101,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.80:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.84:DX
GRAPHICS 3 .80 .84 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0102,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.70:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.74:DX
```

```
GRAPHICS 3 .70 .74 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0103,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.60:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.64:DX
GRAPHICS 3 .60 .64 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0104,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.50:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.54:DX
GRAPHICS 3 .50 .54 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0105,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.40:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.44:DX
GRAPHICS 3 .40 .44 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0106,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.30:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.34:DX
GRAPHICS 3 .30 .34 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0107,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.20:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.23:DX
GRAPHICS 3 .20 .23 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0108,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.10:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.12:DX
GRAPHICS 3 .10 .12 MS1
  ... the command in full is GRAPHICS_PLOT
LABEL AA
  ... the command in full is LABEL_DATA

$
$ Enthalpy of mixing at 1773 K (reference state: liquid)
TABLE_HEAD 110
CREATE_NEW_EQUILIBRIUM 0110,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.9
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT  HMR(LIQ)=-1964:DH
GRAPHICS 2 .9 -1964 MS2
  ... the command in full is GRAPHICS_PLOT
LABEL AH
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0111,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.8
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT  HMR(LIQ)=-3500:DH
GRAPHICS 2 .8 -3500 MS2
  ... the command in full is GRAPHICS_PLOT
LABEL AH
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0112,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.7
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT  HMR(LIQ)=-4588:DH
GRAPHICS 2 .7 -4588 MS2
  ... the command in full is GRAPHICS_PLOT
LABEL AH
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0113,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.6
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT  HMR(LIQ)=-5239:DH
GRAPHICS 2 .6 -5239 MS2
  ... the command in full is GRAPHICS_PLOT
LABEL AH
  ... the command in full is LABEL_DATA
SET_ALL_START Y
  ... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0114,1
CHANGE_STATUS PHASE LIQ=FIX 1
```

```
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.5
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-5454:DH
 GRAPHICS 2 .5 -5454 MS2
   ... the command in full is GRAPHICS_PLOT
 LABEL AH
   ... the command in full is LABEL_DATA
 SET_ALL_START Y
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0115,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.4
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-5233:DH
 GRAPHICS 2 .4 -5233 MS2
   ... the command in full is GRAPHICS_PLOT
 LABEL AH
   ... the command in full is LABEL_DATA
 SET_ALL_START Y
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0116,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.3
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-4575:DH
 GRAPHICS 2 .3 -4575 MS2
   ... the command in full is GRAPHICS_PLOT
 LABEL AH
   ... the command in full is LABEL_DATA
 SET_ALL_START Y
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0117,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.2
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-3481:DH
 GRAPHICS 2 .2 -3481 MS2
   ... the command in full is GRAPHICS_PLOT
 LABEL AH
   ... the command in full is LABEL_DATA
 SET_ALL_START Y
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0118,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.1
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-1950:DH
 GRAPHICS 2 .1 -1950 MS2
   ... the command in full is GRAPHICS_PLOT
 LABEL AH
   ... the command in full is LABEL_DATA
 SET_ALL_START Y
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set

 $
 $ Heat of melting for the compound. T=1341. H(liq)-H(A2B)=3727 J/mol.
 $ This datum has already been used.
 $
 $ Do not forget the following line!
 SAVE_WORKSPACES
PARROT:
PARROT: @@
PARROT: @@ Next file shows how to guess rough start guess of the coefficients
PARROT: @@ and run the actual assessment. The values below are the final result.
PARROT: @@ S-O-V 1 20450,,,,,,
PARROT: @@ S-O-V 2 -30.386,,,,,,,
PARROT: @@ S-O-V 3 0.131,,,,,,
PARROT: @@ S-O-V 11 -21817,,,,,
PARROT: @@ S-O-V 12 15.34,,,,,,,,
PARROT: @@ S-O-V 15 24212,,,,,,
PARROT: @@ S-O-V 16 -8.328,,,,,,,,
PARROT: @@ S-O-V 17 3105,,,,,,
PARROT: @@ S-O-V 19 22030,,,,,,
PARROT: @@ S-O-V 20 -6.981,,,,,,,,
PARROT: @@ save the start guess on the work file
PARROT: s-o-v 1 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: s-o-v 2 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: s-o-v 11 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: s-o-v 12 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: s-o-v 15 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: s-o-v 16 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: s-o-v 17 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: s-o-v 19 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: s-o-v 20 0
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT:
PARROT: save
   ... the command in full is SAVE_PARROT_WORKSPACES
PARROT: @@ Now executing tcex36b.TCM to continue the assessment example
PARROT:Hit RETURN to continue
PARROT: mac tcex36b.TCM
   ... the command in full is MACRO_FILE_OPEN
PARROT: s-s-f tcex36
   ... the command in full is SET_STORE_FILE
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
```

```
   ... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1   TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT: @@ Set alt mode to start
PARROT: s-alt Y
   ... the command in full is SET_ALTERNATE_MODE
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV *alt*  1.0  1193.0      LIQUID A2B BCC
   2 AINV *alt*  1.0  1341.0      LIQUID A2B
   3 AINV *alt*  1.0  1049.0      LIQUID A2B BCC
   4 AINV *alt*  1.0  1203.0      LIQUID BCC FCC
   5 AINV *alt*  1.0   726.0      A2B BCC BCC#2
   6 AINV *alt*  1.0   726.0      BCC BCC#2
 Failed using alternate for FCC#1                     setting weight to zero
  10 ALF  *alt*  1.0  1594.0      LIQUID FCC
 Failed using alternate for FCC#1                     setting weight to zero
  11 ALF  *alt*  1.0  1548.0      LIQUID FCC
 Failed using alternate for FCC#1                     setting weight to zero
  12 ALF  *alt*  1.0  1499.0      LIQUID FCC
 Failed using alternate for FCC#1                     setting weight to zero
  13 ALF  *alt*  1.0  1438.0      LIQUID FCC
  20 ATIE *alt*  1.0  1413.0      LIQUID FCC
  21 ATIE *alt*  1.0  1337.0      LIQUID FCC
  22 ATIE *alt*  1.0  1213.0      LIQUID FCC
  23 ATIE *alt*  1.0  1100.0      LIQUID BCC
 100 AA      5   1.    1573.0      LIQUID
 101 AA      4   1.    1573.0      LIQUID
 102 AA      2   1.    1573.0      LIQUID
 103 AA      3   1.    1573.0      LIQUID
 104 AA      4   1.    1573.0      LIQUID
 105 AA      6   1.    1573.0      LIQUID
 106 AA      8   1.    1573.0      LIQUID
 107 AA      9   1.    1573.0      LIQUID
 108 AA     11   1.    1573.0      LIQUID
 110 AH      8   1.    1773.0      LIQUID
 111 AH      6   1.    1773.0      LIQUID
 112 AH      5   1.    1773.0      LIQUID
 113 AH      3   1.    1773.0      LIQUID
 114 AH      2   1.    1773.0      LIQUID
 115 AH      3   1.    1773.0      LIQUID
 116 AH      5   1.    1773.0      LIQUID
 117 AH      7   1.    1773.0      LIQUID
 118 AH      8   1.    1773.0      LIQUID
 Number of alternate equilibria                      14
ED_EXP: @@ Equilibra with label ALF cannot use alt mode
ED_EXP: s-we 0 alf
   ... the command in full is SET_WEIGHT
 Changed weight on                      4  equilibria.
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
 118 AH      2   1.    1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes of weights before leaving editor
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ Optimize zero times as a check
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20: 7




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==
```

```
 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   1.22023362E+03
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   3.21114110E+01

 Number of alternate equilibria                     10

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                      1.81
   2 Alternate equilibrium calc                                      0.39
2 HTR=3727                       1.5333E+04  5.00E+02  1.1606E+04   23.21    *
   3 Alternate equilibrium calc                                      1.32
   4 Alternate equilibrium calc                                      1.56
   5 Alternate equilibrium calc                                      4.14
   6 Alternate equilibrium calc                                      3.83
  20 Alternate equilibrium calc                                      0.87
  21 Alternate equilibrium calc                                      0.97
  22 Alternate equilibrium calc                                      1.14
  23 Alternate equilibrium calc                                      1.20
100 ACR(B)=0.94                  0.9382      2.89E-02 -1.8474E-03 -6.3948E-02
101 ACR(B)=0.84                  0.8339      2.89E-02 -6.0866E-03 -0.2107
102 ACR(B)=0.74                  0.7297      2.89E-02 -1.0326E-02 -0.3574
103 ACR(B)=0.64                  0.6254      2.89E-02 -1.4565E-02 -0.5042
104 ACR(B)=0.54                  0.5212      2.89E-02 -1.8804E-02 -0.6509
105 ACR(B)=0.44                  0.4170      2.89E-02 -2.3043E-02 -0.7976
106 ACR(B)=0.34                  0.3127      2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23                  0.2085      2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12                  0.1042      2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964             0.000      5.00E+02   1964.       3.928
111 HMR(LIQUID)=-3500             0.000      5.00E+02   3500.       7.000    *
112 HMR(LIQUID)=-4588             0.000      5.00E+02   4588.       9.176    *
113 HMR(LIQUID)=-5239           -3.6380E-12  5.00E+02   5239.       10.48    *
114 HMR(LIQUID)=-5454            1.8190E-12  5.00E+02   5454.       10.91    *
115 HMR(LIQUID)=-5233            1.8190E-12  5.00E+02   5233.       10.47    *
116 HMR(LIQUID)=-4575           -1.8190E-12  5.00E+02   4575.       9.150    *
117 HMR(LIQUID)=-3481             0.000      5.00E+02   3481.       6.962    *
118 HMR(LIQUID)=-1950           -1.8190E-12  5.00E+02   1950.       3.900


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Note only one error from alternate calculations. This error represents
PARROT: @@ the difference in chemical potentials of the phases.
PARROT: @@ Experiments with just one phase is calculated as normal.
PARROT: @@ Next command supresses listing of parameters.
PARROT: s-o-l 1 Y Y N n N
   ... the command in full is SET_OUTPUT_LEVELS
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT
```

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           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20: 7



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =    0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   1.22023362E+03
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   3.21114110E+01

 Number of alternate equilibria                     10


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                      1.81
   2 Alternate equilibrium calc                                      0.39
2 HTR=3727                      1.5333E+04  5.00E+02  1.1606E+04   23.21    *
   3 Alternate equilibrium calc                                      1.32
   4 Alternate equilibrium calc                                      1.56
   5 Alternate equilibrium calc                                      4.14
   6 Alternate equilibrium calc                                      3.83
  20 Alternate equilibrium calc                                      0.87
  21 Alternate equilibrium calc                                      0.97
  22 Alternate equilibrium calc                                      1.14
  23 Alternate equilibrium calc                                      1.20
100 ACR(B)=0.94                 0.9382      2.89E-02 -1.8474E-03 -6.3948E-02
101 ACR(B)=0.84                 0.8339      2.89E-02 -6.0866E-03 -0.2107
102 ACR(B)=0.74                 0.7297      2.89E-02 -1.0326E-02 -0.3574
103 ACR(B)=0.64                 0.6254      2.89E-02 -1.4565E-02 -0.5042
104 ACR(B)=0.54                 0.5212      2.89E-02 -1.8804E-02 -0.6509
105 ACR(B)=0.44                 0.4170      2.89E-02 -2.3043E-02 -0.7976
106 ACR(B)=0.34                 0.3127      2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23                 0.2085      2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12                 0.1042      2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964            0.000      5.00E+02   1964.       3.928
111 HMR(LIQUID)=-3500            0.000      5.00E+02   3500.       7.000    *
112 HMR(LIQUID)=-4588            0.000      5.00E+02   4588.       9.176    *
113 HMR(LIQUID)=-5239          -3.6380E-12  5.00E+02   5239.       10.48    *
114 HMR(LIQUID)=-5454           1.8190E-12  5.00E+02   5454.       10.91    *
115 HMR(LIQUID)=-5233           1.8190E-12  5.00E+02   5233.       10.47    *
116 HMR(LIQUID)=-4575          -1.8190E-12  5.00E+02   4575.       9.150    *
117 HMR(LIQUID)=-3481            0.000      5.00E+02   3481.       6.962    *
118 HMR(LIQUID)=-1950          -1.8190E-12  5.00E+02   1950.       3.900


PARROT:
PARROT: @@ Now optimize
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    1.22023362E+03
  1  0.0000E+00   2  0.0000E+00   3  0.0000E+00   4  0.0000E+00   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    1.22023056E+03
  1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  0.0000E+00   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    1.22026107E+03
  1  1.0000E-04   2  1.0000E-04   3  0.0000E+00   4  0.0000E+00   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.22023821E+03
  1  1.0000E-04   2  0.0000E+00   3  1.0000E-04   4  0.0000E+00   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21985896E+03
  1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21985855E+03
  1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00
```

```
    AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21952877E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  1.0000E-04   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

    AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21952862E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  1.0000E-04   7  1.0000E-04   8  0.0000E+00   9  0.0000E+00

    AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21952856E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  1.0000E-04   7  1.0000E-04   8  1.0000E-04   9  0.0000E+00

    AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21945175E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  1.0000E-04   7  1.0000E-04   8  1.0000E-04   9  1.0000E-04

    AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21347918E+03
 1  1.1575E-04   2 -1.5562E-04   3 -3.9485E-05   4  1.9219E-03   5  1.0209E-04
 6  1.7933E-03   7  1.0073E-04   8  1.0031E-04   9  4.9349E-04

    AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.20857820E+03
 1  5.7604E-04   2 -2.8000E-04   3 -5.5554E-04   4  2.9761E-04   5  1.0310E-03
 6  3.2119E-03   7  1.5940E-04   8  5.6559E-04   9  8.6813E-04

    AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.20419111E+03
 1  1.7517E-03   2 -4.0933E-04   3 -1.8427E-03   4  1.7341E-03   5  1.9072E-03
 6  4.5182E-03   7  3.6464E-04   8 -3.6442E-03   9  1.2034E-03

    AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    1.20018978E+03
 1  4.9647E-03   2 -5.3990E-04   3 -5.3422E-03   4  4.2170E-04   5  1.3348E-03
 6  5.8647E-03   7  1.0916E-03   8 -1.0101E-02   9  1.5910E-03

    AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    1.19656103E+03
 1  8.7053E-03   2 -6.5937E-04   3 -9.4048E-03   4  1.6713E-03   5  2.0976E-03
 6  6.9625E-03   7  1.8270E-03   8 -2.5618E-02   9  1.9085E-03

    AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    1.19290093E+03
 1  1.6702E-02   2 -7.8966E-04   3 -1.8062E-02   4  5.3932E-04   5  2.8050E-03
 6  8.1461E-03   7  3.5323E-03   8 -5.6536E-02   9  2.2985E-03

    AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    1.18895829E+03
 1  2.9858E-02   2 -9.1157E-04   3 -3.2288E-02   4  1.6316E-03   5  6.0830E-03
 6  9.0741E-03   7  6.1592E-03   8 -1.1985E-01   9  2.6324E-03

    AT THE   17 TH ITERATION WE HAVE THE SUM OF SQUARES    1.18371835E+03
 1  5.7117E-02   2 -1.0621E-03   3 -6.1739E-02   4  6.6639E-04   5  1.1597E-02
 6  1.0112E-02   7  1.1749E-02   8 -2.4612E-01   9  3.0842E-03

    AT THE   18 TH ITERATION WE HAVE THE SUM OF SQUARES    1.17576307E+03
 1  1.0981E-01   2 -1.2302E-03   3 -1.1865E-01   4  1.6444E-03   5  2.3336E-02
 6  1.0904E-02   7  2.2419E-02   8 -4.9950E-01   9  3.5580E-03

    AT THE   19 TH ITERATION WE HAVE THE SUM OF SQUARES    1.17580508E+03
 1  1.0990E-01   2 -1.2331E-03   3 -1.1866E-01   4  1.6767E-03   5  2.3332E-02
 6  1.0908E-02   7  2.2420E-02   8 -4.9948E-01   9  3.5631E-03

    AT THE   20 TH ITERATION WE HAVE THE SUM OF SQUARES    1.17576898E+03
 1  1.0981E-01   2 -1.1307E-03   3 -1.1865E-01   4  1.6454E-03   5  2.3336E-02
 6  1.0913E-02   7  2.2419E-02   8 -4.9950E-01   9  3.5581E-03

    AT THE   21 TH ITERATION WE HAVE THE SUM OF SQUARES    1.17573278E+03
 1  1.0983E-01   2 -1.2301E-03   3 -1.1856E-01   4  1.6164E-03   5  2.3339E-02
 6  1.0901E-02   7  2.2419E-02   8 -4.9952E-01   9  3.5536E-03

    AT THE   22 TH ITERATION WE HAVE THE SUM OF SQUARES    1.15839209E+03
 1  2.4518E-01   2 -1.5171E-03   3 -2.6482E-01   4  8.9861E-04   5  8.1375E-02
 6  1.1834E-02   7  4.7658E-02   8 -9.8754E-01   9  4.3315E-03

    AT THE   23 TH ITERATION WE HAVE THE SUM OF SQUARES    1.15852291E+03
 1  2.4519E-01   2 -1.5109E-03   3 -2.6483E-01   4  8.8627E-04   5  8.1444E-02
 6  1.1766E-02   7  4.7657E-02   8 -9.8753E-01   9  4.3220E-03

    AT THE   24 TH ITERATION WE HAVE THE SUM OF SQUARES    1.12429808E+03
 1  5.3085E-01   2 -1.9804E-03   3 -5.7319E-01   4  1.9224E-03   5  3.5639E-01
 6  1.2271E-02   7  9.3910E-02   8 -1.9219E+00   9  5.3987E-03

    AT THE   25 TH ITERATION WE HAVE THE SUM OF SQUARES    1.12430368E+03
 1  5.3084E-01   2 -1.9806E-03   3 -5.7319E-01   4  1.9278E-03   5  3.5639E-01
 6  1.2272E-02   7  9.4010E-02   8 -1.9219E+00   9  5.3997E-03

    AT THE   26 TH ITERATION WE HAVE THE SUM OF SQUARES    1.05801747E+03
 1  1.1108E+00   2 -2.8497E-03   3 -1.1990E+00   4  1.6568E-03   5  1.0413E+00
 6  1.2349E-02   7  1.7987E-01   8 -3.7400E+00   9  7.2585E-03

    AT THE   27 TH ITERATION WE HAVE THE SUM OF SQUARES    1.05799597E+03
 1  1.1108E+00   2 -2.8479E-03   3 -1.1990E+00   4  1.6562E-03   5  1.0413E+00
 6  1.2329E-02   7  1.7987E-01   8 -3.7401E+00   9  7.3562E-03

    AT THE   28 TH ITERATION WE HAVE THE SUM OF SQUARES    9.32316420E+02
 1  2.2754E+00   2 -4.5180E-03   3 -2.4557E+00   4  3.1330E-03   5  2.5155E+00
 6  1.1608E-02   7  3.4709E-01   8 -7.3322E+00   9  1.0723E-02

    AT THE   29 TH ITERATION WE HAVE THE SUM OF SQUARES    9.32175579E+02
 1  2.2754E+00   2 -4.5239E-03   3 -2.4557E+00   4  3.0908E-03   5  2.5156E+00
 6  1.1674E-02   7  3.4709E-01   8 -7.3322E+00   9  1.0740E-02

    AT THE   30 TH ITERATION WE HAVE THE SUM OF SQUARES    9.32266522E+02
 1  2.2754E+00   2 -4.5260E-03   3 -2.4557E+00   4  3.1696E-03   5  2.5156E+00
 6  1.1696E-02   7  3.4708E-01   8 -7.3322E+00   9  1.0745E-02

*** ERROR RETURN FROM VA05A BECAUSE THERE HAVE BEEN   30 CALLS OF CALFUN

   THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   30 iterations
 1  2.2754E+00   2 -4.5239E-03   3 -2.4557E+00   4  3.0908E-03   5  2.5156E+00
 6  1.1674E-02   7  3.4709E-01   8 -7.3322E+00   9  1.0740E-02

 1  2.7586E-01   2  2.7586E-01   3 -2.3479E-02   4 -2.9092E-01   5 -1.4825E-01
 6 -2.4894E-01   7  2.0604E+01   8  1.1427E-01   9  1.1427E-01  10 -2.1551E-01
11 -1.4793E-01  12  6.1401E-02  13 -4.3625E-02  14 -7.7890E-01  15 -8.0449E-02
16  4.8856E-01  17  4.8856E-01  18 -7.3181E-01  19  1.4636E+00  20 -7.3181E-01
21  1.4636E+00  22 -4.1620E-01  23 -1.1022E-02  24 -5.4162E-01  25 -2.8760E-02
26 -7.6572E-01  27 -7.3156E-02  28 -1.2544E-01  29 -1.0373E-01  30 -4.2177E-03
31  2.5902E-03  32  6.6372E-02  33  1.4719E-01  34  2.0341E-01  35  1.9322E-01
36  7.6393E-02  37  1.5206E-01  38  3.2168E-02  39  3.4860E+00  40  6.2142E+00
41  8.1446E+00  42  9.2993E+00  43  9.6801E+00  44  9.2873E+00  45  8.1186E+00
```

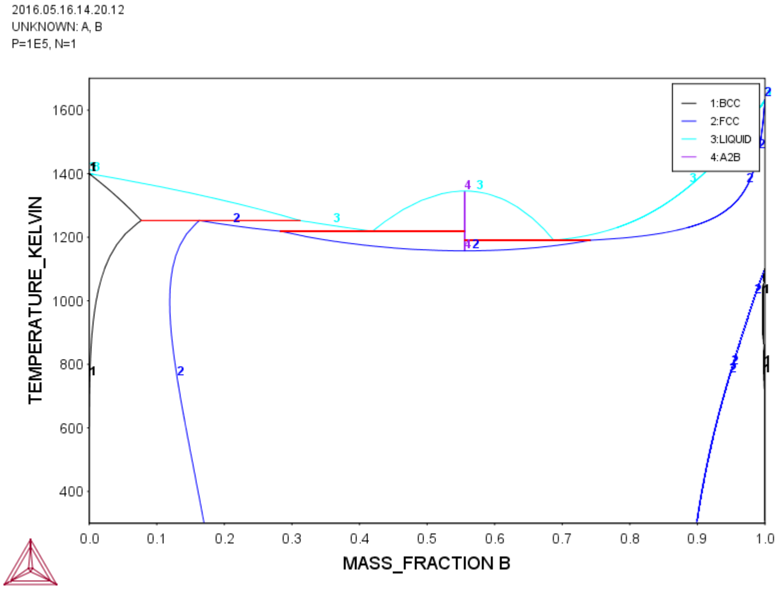
```
 46  6.1762E+00   47  3.4580E+00

               THE SUM OF SQUARES IS   9.32175579E+02
PARROT: cont 30
   ... the command in full is CONTINUE_OPTIMIZATION
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A
    Optimization continuing with same Jacobian


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    6.42378436E+02
  1  5.3285E+00   2 -8.7738E-03   3 -5.7409E+00   4  4.7675E-03   5  5.1386E+00
  6  9.8927E-03   7  8.7846E-01   8 -1.4032E+01   9  1.6957E-02

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    3.93287140E+02
  1  8.5798E+00   2 -1.3317E-02   3 -9.2391E+00   4  7.4937E-03   5  8.0040E+00
  6  7.9956E-03   7  1.4404E+00   8 -2.1386E+01   9  2.3783E-02

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    2.09581259E+02
  1  1.1739E+01   2 -1.7636E-02   3 -1.2638E+01   4  9.3818E-03   5  1.0889E+01
  6  5.4398E-03   7  1.9808E+00   8 -2.8820E+01   9  3.0390E-02

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.80919629E+01
  1  1.7814E+01   2 -2.5900E-02   3 -1.9174E+01   4  1.3734E-02   5  1.6703E+01
  6 -6.1201E-06   7  3.0058E+00   8 -4.3892E+01   9  4.3587E-02

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    9.80059382E-01
  1  2.0269E+01   2 -2.9190E-02   3 -2.1813E+01   4  1.5556E-02   5  1.9856E+01
  6 -3.2628E-03   7  3.3757E+00   8 -5.2038E+01   9  5.0439E-02

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    4 iterations
  1  2.0269E+01   2 -2.9190E-02   3 -2.1813E+01   4  1.5556E-02   5  1.9856E+01
  6 -3.2628E-03   7  3.3757E+00   8 -5.2038E+01   9  5.0439E-02

  1 -1.6298E-03   2 -1.6298E-03   3  1.8275E-04   4  1.5454E-01   5  1.3483E-01
  6 -1.3372E-01   7  5.3414E-03   8 -1.9207E-03   9 -1.9207E-03  10  5.9902E-02
 11 -5.3043E-03  12  1.0919E-01  13 -3.1490E-03  14 -3.7871E-01  15 -1.5089E-02
 16  2.6188E-02  17  2.6188E-02  18 -1.0466E-01  19  6.6482E-02  20 -1.0466E-01
 21  6.6482E-02  22  4.7595E-01  23  4.3175E-03  24  1.7990E-01  25 -3.8166E-04
 26 -3.4079E-01  27 -1.0881E-02  28  7.4581E-02  29 -2.7851E-03  30  2.1227E-03
 31  2.5569E-02  32  1.1253E-01  33  2.1861E-01  34  2.9732E-01  35  3.0190E-01
 36  1.8750E-01  37  2.4843E-01  38  9.3003E-02  39  1.7059E-03  40  1.9922E-02
 41  1.4647E-02  42  7.8823E-03  43  1.6274E-03  44 -4.1177E-03  45 -1.1353E-02
 46 -1.8078E-02  47 -2.6294E-02

               THE SUM OF SQUARES IS   9.80059382E-01
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20: 8




 *** OPTIMIZATION ERROR. TOO MANY ITERATIONS ***
     NUMBER OF ITERATIONS:    5


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   30    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1   TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02691580E+04    0.00000000E+00    1.00000000E+03    1.60588759E+00
 V2     -2.91902505E+01    0.00000000E+00    1.00000000E+03    1.00991507E-02
 V11    -2.18127452E+04    0.00000000E+00    1.00000000E+03    8.65821611E-01
 V12     1.55559572E+01    0.00000000E+00    1.00000000E+03    2.63407916E-03
 V15     1.98562648E+04    0.00000000E+00    1.00000000E+03    1.43531758E+01
 V16    -3.26280484E+00    0.00000000E+00    1.00000000E+03    1.71198002E-02
 V17     3.37569790E+03    0.00000000E+00    1.00000000E+03    4.53503022E+00
 V19    -5.20381430E+04    0.00000000E+00    1.00000000E+03    3.15147730E+01
 V20     5.04393965E+01    0.00000000E+00    1.00000000E+03    2.47939786E-02

 NUMBER OF OPTIMIZING VARIABLES :    9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.22023362E+03 TO    9.80059382E-01
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   2.57910364E-02

 Number of alternate equilibria                     10


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                       0.15
   2 Alternate equilibrium calc                                       0.19
2 HTR=3727                        3730.      5.00E+02   2.671      5.3414E-03
   3 Alternate equilibrium calc                                       0.06
   4 Alternate equilibrium calc                                       0.39
   5 Alternate equilibrium calc                                       0.13
   6 Alternate equilibrium calc                                       0.12
  20 Alternate equilibrium calc                                       0.48
  21 Alternate equilibrium calc                                       0.18
  22 Alternate equilibrium calc                                       0.34
  23 Alternate equilibrium calc                                       0.07
100 ACR(B)=0.94                  0.9401      2.84E-02  6.0229E-05  2.1227E-03
```

```
101 ACR(B)=0.84                  0.8407      2.80E-02  7.1694E-04  2.5569E-02
102 ACR(B)=0.74                  0.7431      2.79E-02  3.1371E-03  0.1125
103 ACR(B)=0.64                  0.6461      2.79E-02  6.0969E-03  0.2186
104 ACR(B)=0.54                  0.5483      2.81E-02  8.3480E-03  0.2973
105 ACR(B)=0.44                  0.4486      2.85E-02  8.5911E-03  0.3019
106 ACR(B)=0.34                  0.3454      2.90E-02  5.4464E-03  0.1875
107 ACR(B)=0.23                  0.2374      2.99E-02  7.4229E-03  0.2484
108 ACR(B)=0.12                  0.1229      3.10E-02  2.8826E-03  9.3003E-02
110 HMR(LIQUID)=-1964            -1963.      5.00E+02  0.8529      1.7059E-03
111 HMR(LIQUID)=-3500            -3490.      5.00E+02   9.961      1.9922E-02
112 HMR(LIQUID)=-4588            -4581.      5.00E+02   7.324      1.4647E-02
113 HMR(LIQUID)=-5239            -5235.      5.00E+02   3.941      7.8823E-03
114 HMR(LIQUID)=-5454            -5453.      5.00E+02  0.8137      1.6274E-03
115 HMR(LIQUID)=-5233            -5235.      5.00E+02  -2.059     -4.1177E-03
116 HMR(LIQUID)=-4575            -4581.      5.00E+02  -5.676     -1.1353E-02
117 HMR(LIQUID)=-3481            -3490.      5.00E+02  -9.039     -1.8078E-02
118 HMR(LIQUID)=-1950            -1963.      5.00E+02  -13.15     -2.6294E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ The liquid data fitted reasonable, fix its parameters to simplify
PARROT: l-p-d liq
   ... the command in full is LIST_PHASE_DATA


 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T
PARROT: s-f-v 11-14
   ... the command in full is SET_FIX_VARIABLE
PARROT: @@ Rescale the start values of the parameters to current values
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: l-a-v
   ... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02691580E+04    2.02691580E+04    2.02691580E+04    0.00000000E+00
 V2     -2.91902505E+01   -2.91902505E+01   -2.91902505E+01    0.00000000E+00
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     1.98562648E+04    1.98562648E+04    1.98562648E+04    0.00000000E+00
 V16    -3.26280484E+00   -3.26280484E+00   -3.26280484E+00    0.00000000E+00
 V17     3.37569790E+03    3.37569790E+03    3.37569790E+03    0.00000000E+00
 V19    -5.20381430E+04   -5.20381430E+04   -5.20381430E+04    0.00000000E+00
 V20     5.04393965E+01    5.04393965E+01    5.04393965E+01    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT:Hit RETURN to continue
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
```

```
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   8.907E-02  3.100E+02
     BCC
  ** FCC
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   8.956E-02  3.000E+02
     BCC
  ** FCC
 Calculated.                     29  equilibria

 Phase region boundary   3 at:   1.213E-01  1.253E+03
  ** LIQUID
     BCC
  ** FCC

 Phase region boundary   4 at:   2.038E-01  1.253E+03
  ** LIQUID
     BCC
 Calculated                     26  equilibria

 Phase region boundary   5 at:   2.413E-01  1.253E+03
  ** LIQUID
     FCC
 Calculated.                      6  equilibria

 Phase region boundary   6 at:   3.546E-01  1.219E+03
  ** LIQUID
  ** A2B
     FCC

 Phase region boundary   7 at:   4.342E-01  1.219E+03
  ** A2B
     FCC
 Calculated.                     24  equilibria

 Phase region boundary   8 at:   6.572E-01  1.191E+03
  ** LIQUID
  ** A2B
     FCC

 Phase region boundary   9 at:   7.154E-01  1.191E+03
  ** LIQUID
     FCC
 Calculated                     43  equilibria

 Phase region boundary  10 at:   6.257E-01  1.191E+03
  ** LIQUID
     A2B
 Calculated.                     23  equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   8.907E-02  3.100E+02
     BCC
  ** FCC
 Calculated.                     28  equilibria
 Terminating at known equilibrium

 Phase region boundary  12 at:   8.907E-02  3.100E+02
     BCC
  ** FCC
 Calculated..                      2  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  13 at:   8.907E-02  3.100E+02
     BCC
  ** FCC
 Calculated.                     28  equilibria
 Terminating at known equilibrium

 Phase region boundary  14 at:   4.559E-01  1.196E+03
  ** A2B
     FCC
 Calculated.                      3  equilibria
 Terminating at known equilibrium
```

```
Phase region boundary  15 at:   4.559E-01  1.196E+03
 ** A2B
    FCC
Calculated.                     21  equilibria
Terminating at known equilibrium

Phase region boundary  16 at:   6.122E-01  1.168E+03
 ** A2B
    FCC
Calculated.                     16  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   6.122E-01  1.168E+03
 ** A2B
    FCC
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   9.533E-01  3.100E+02
    BCC
 ** FCC
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary  19 at:   9.530E-01  3.000E+02
    BCC
 ** FCC
Calculated                     31  equilibria

Phase region boundary  20 at:   9.533E-01  3.100E+02
    BCC
 ** FCC
Calculated                     29  equilibria

Phase region boundary  21 at:   9.533E-01  3.100E+02
    BCC
 ** FCC
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   9.533E-01  3.100E+02
    BCC
 ** FCC
Calculated                     29  equilibria

Phase region boundary  23 at:   6.769E-02  7.700E+02
    BCC
 ** FCC
Calculated..                     15  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   6.769E-02  7.700E+02
    BCC
 ** FCC
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   9.745E-01  7.700E+02
    BCC
 ** FCC
Calculated..                     15  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  26 at:   9.745E-01  7.700E+02
    BCC
 ** FCC
Calculated                     18  equilibria

Phase region boundary  27 at:   1.086E-01  1.230E+03
    BCC
 ** FCC
Calculated..                     28  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:   1.086E-01  1.230E+03
    BCC
 ** FCC
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   8.359E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   8.359E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                     37  equilibria

Phase region boundary  31 at:   6.124E-03  1.396E+03
    LIQUID
 ** BCC
Calculated                     11  equilibria

Phase region boundary  32 at:   6.124E-03  1.396E+03
    LIQUID
 ** BCC
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   2.658E-01  1.244E+03
    LIQUID
 ** FCC
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   2.658E-01  1.244E+03
    LIQUID
 ** FCC
Calculated.                      5  equilibria
```

```
 Terminating at known equilibrium

 Phase region boundary  35 at:   6.122E-01  1.246E+03
     LIQUID
  ** A2B
 Calculated.                     13  equilibria
 Terminating at known equilibrium

 Phase region boundary  36 at:   6.122E-01  1.246E+03
     LIQUID
  ** A2B
 Calculated.                      4  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   9.944E-01  1.601E+03
     LIQUID
  ** FCC
 Calculated.                     33  equilibria
 Terminating at known equilibrium

 Phase region boundary  38 at:   9.944E-01  1.601E+03
     LIQUID
  ** FCC
 Calculated                     12  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                      0  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use     824 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


     AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    9.80059382E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    9.80052014E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    9.80051985E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    9.79978216E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    9.79978097E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    9.79978348E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
```

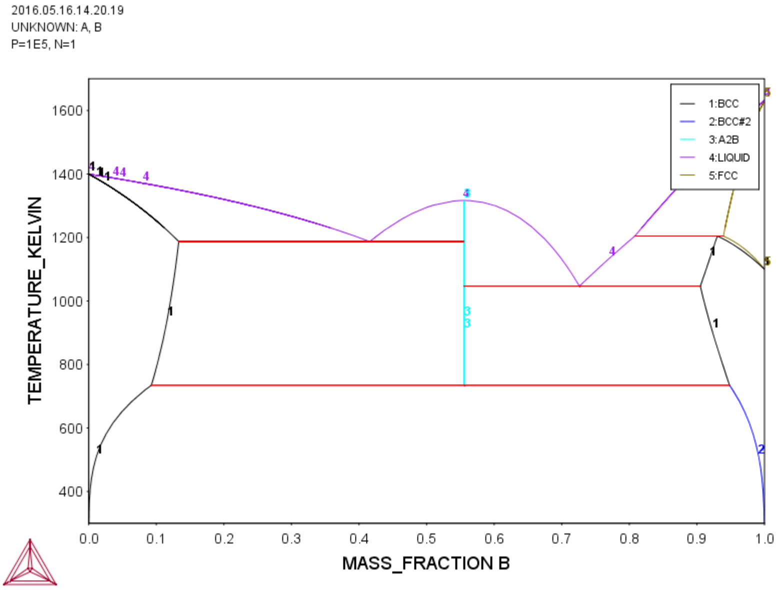
```
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    9.80052308E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    9.79979005E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    9.74568992E-01
  1  1.0007E+00   2  1.0001E+00   3  1.0074E+00   4  1.0001E+00   5  9.9998E-01
  6  9.9266E-01   7  1.0000E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    9.68323516E-01
  1  1.0001E+00   2  9.9993E-01   3  1.0086E+00   4  1.0048E+00   5  9.9962E-01
  6  9.8903E-01   7  9.9159E-01

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    9.58298224E-01
  1  1.0012E+00   2  9.9951E-01   3  1.0105E+00   4  1.0150E+00   5  9.9882E-01
  6  9.7286E-01   7  9.8384E-01

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    9.36475670E-01
  1  9.9970E-01   2  9.9934E-01   3  1.0140E+00   4  1.0400E+00   5  9.9747E-01
  6  9.4967E-01   7  9.6043E-01

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    8.96558227E-01
  1  1.0019E+00   2  9.9883E-01   3  1.0209E+00   4  1.0903E+00   5  9.9477E-01
  6  8.9661E-01   7  9.2172E-01

      AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    8.20182625E-01
  1  9.9941E-01   2  9.9846E-01   3  1.0352E+00   4  1.1942E+00   5  9.8966E-01
  6  7.9747E-01   7  8.3959E-01

      AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    6.87461582E-01
  1  1.0018E+00   2  9.9752E-01   3  1.0636E+00   4  1.4027E+00   5  9.7946E-01
  6  5.9608E-01   7  6.7987E-01

      AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    6.87514987E-01
  1  1.0019E+00   2  9.9752E-01   3  1.0636E+00   4  1.4027E+00   5  9.7946E-01
  6  5.9609E-01   7  6.7985E-01

      AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    6.87460994E-01
  1  1.0018E+00   2  9.9762E-01   3  1.0636E+00   4  1.4027E+00   5  9.7946E-01
  6  5.9608E-01   7  6.7987E-01

      AT THE   17 TH ITERATION WE HAVE THE SUM OF SQUARES    4.93890786E-01
  1  9.9983E-01   2  9.9617E-01   3  1.1210E+00   4  1.8222E+00   5  9.5929E-01
  6  1.9649E-01   7  3.5984E-01

      AT THE   18 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83968704E-01
  1  1.0003E+00   2  9.9394E-01   3  1.2080E+00   4  2.4586E+00   5  9.2882E-01
  6 -4.0863E-01   7 -1.2364E-01

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   18 iterations
  1  1.0003E+00   2  9.9394E-01   3  1.2080E+00   4  2.4586E+00   5  9.2882E-01
  6 -4.0863E-01   7 -1.2364E-01

  1  5.6826E-03   2  5.6826E-03   3 -5.2705E-04   4 -1.0121E-03   5  1.2997E-01
  6 -1.3615E-01   7  9.2250E-04   8  5.4224E-03   9  5.4224E-03  10  5.3339E-04
 11 -6.9115E-03  12  2.1376E-03  13 -5.6501E-03  14  2.0876E-03  15 -5.3921E-03
 16  9.5282E-03  17  9.5282E-03  18  2.1204E-04  19 -3.0973E-03  20  2.1204E-04
 21 -3.0973E-03  22 -2.1113E-03  23 -3.4457E-04  24  3.5839E-03  25 -3.0619E-03
 26 -3.2846E-03  27 -2.5884E-03  28 -6.7137E-04  29 -4.9774E-03  30  2.1227E-03
 31  2.5569E-02  32  1.1253E-01  33  2.1861E-01  34  2.9732E-01  35  3.0190E-01
 36  1.8750E-01  37  2.4843E-01  38  9.3003E-02  39  1.7059E-03  40  1.9922E-02
 41  1.4647E-02  42  7.8823E-03  43  1.6274E-03  44 -4.1177E-03  45 -1.1353E-02
 46 -1.8078E-02  47 -2.6294E-02

               THE SUM OF SQUARES IS   3.83968704E-01
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use     824 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83968704E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    3.83970580E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    3.83968793E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    3.83969329E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83968753E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83968710E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83968800E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83968718E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0001E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    7 iterations
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00
```

```
  1  5.6826E-03   2  5.6826E-03   3 -5.2705E-04   4 -1.0121E-03   5  1.2997E-01
  6 -1.3615E-01   7  9.2250E-04   8  5.4224E-03   9  5.4224E-03  10  5.3339E-04
 11 -6.9115E-03  12  2.1376E-03  13 -5.6501E-03  14  2.0876E-03  15 -5.3921E-03
 16  9.5282E-03  17  9.5282E-03  18  2.1204E-04  19 -3.0973E-03  20  2.1204E-04
 21 -3.0973E-03  22 -2.1113E-03  23 -3.4457E-04  24  3.5839E-03  25 -3.0619E-03
 26 -3.2846E-03  27 -2.5884E-03  28 -6.7137E-04  29 -4.9774E-03  30  2.1227E-03
 31  2.5569E-02  32  1.1253E-01  33  2.1861E-01  34  2.9732E-01  35  3.0190E-01
 36  1.8750E-01  37  2.4843E-01  38  9.3003E-02  39  1.7059E-03  40  1.9922E-02
 41  1.4647E-02  42  7.8823E-03  43  1.6274E-03  44 -4.1177E-03  45 -1.1353E-02
 46 -1.8078E-02  47 -2.6294E-02

               THE SUM OF SQUARES IS   3.83968704E-01
PARROT: @@ No change in the parameters, check the diagram again
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC
  ** BCC#2
 Calculated..                        2  equilibria
 Terminating at axis limit.
```

```
Phase region boundary   2 at:   7.141E-01  3.000E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria

Phase region boundary   3 at:   6.802E-01  7.347E+02
 ** A2B
    BCC
 ** BCC#2

Phase region boundary   4 at:   3.640E-01  7.347E+02
 ** A2B
    BCC
Calculated.                     14  equilibria

Phase region boundary   5 at:   3.781E-01  1.187E+03
 ** LIQUID
 ** A2B
    BCC

Phase region boundary   6 at:   2.888E-01  1.187E+03
 ** LIQUID
    BCC
Calculated                     27  equilibria

Phase region boundary   7 at:   4.898E-01  1.187E+03
 ** LIQUID
    A2B
Calculated.                     26  equilibria

Phase region boundary   8 at:   6.479E-01  1.047E+03
 ** LIQUID
    A2B
 ** BCC

Phase region boundary   9 at:   7.629E-01  1.047E+03
    A2B
 ** BCC
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.250E-01  1.047E+03
    LIQUID
 ** BCC
Calculated.                      9  equilibria

Phase region boundary  11 at:   8.738E-01  1.205E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.791E-01  1.205E+03
    LIQUID
 ** FCC
Calculated                     37  equilibria

Phase region boundary  13 at:   9.347E-01  1.205E+03
    BCC
 ** FCC
Calculated                     26  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
```

```
    BCC#2
Calculated.                      14  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                      14  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.657E-01  7.700E+02
 ** A2B
    BCC
Calculated                      10  equilibria

Phase region boundary  26 at:   3.657E-01  7.700E+02
 ** A2B
    BCC
Calculated.                       3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.657E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.900E-01  7.700E+02
 ** A2B
    BCC
Calculated                      10  equilibria

Phase region boundary  29 at:   7.900E-01  7.700E+02
 ** A2B
    BCC
Calculated.                       3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.900E-01  7.700E+02
 ** A2B
    BCC
Calculated.                       9  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.459E-01  1.230E+03
 ** LIQUID
    BCC
Calculated.                       4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.459E-01  1.230E+03
 ** LIQUID
    BCC
Calculated                      26  equilibria

Phase region boundary  33 at:   8.847E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                       2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.847E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                      29  equilibria

Phase region boundary  35 at:   6.422E-03  1.397E+03
    LIQUID
 ** BCC
Calculated                       9  equilibria

Phase region boundary  36 at:   6.422E-03  1.397E+03
    LIQUID
 ** BCC
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.299E-01  1.244E+03
    LIQUID
 ** BCC
Calculated                      19  equilibria

Phase region boundary  38 at:   2.299E-01  1.244E+03
    LIQUID
 ** BCC
Calculated.                       4  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.219E+03
    LIQUID
 ** A2B
Calculated.                      12  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.122E-01  1.219E+03
    LIQUID
 ** A2B
Calculated.                       7  equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   9.927E-01  1.613E+03
    LIQUID
 ** FCC
Calculated.                      20  equilibria
Terminating at known equilibrium

Phase region boundary  42 at:   9.927E-01  1.613E+03
    LIQUID
 ** FCC
```

```
 Calculated                      13  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                      0  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Turn off alternate mode and try to calculate all equilibria
PARROT: s-alt Y
   ... the command in full is SET_ALTERNATE_MODE
 Alternate calculation is on
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   3   1.    1187.5      LIQUID A2B BCC
   2 AINV   2   1.    1316.7      LIQUID A2B
   3 AINV   3   1.    1047.0      LIQUID A2B BCC
   4 AINV   3   1.    1204.7      LIQUID BCC FCC
   5 AINV   4   1.     734.7      A2B BCC BCC#2
   6 AINV   3   1.     726.0      BCC BCC#2
  10 ALF  < unused >  1594.0      LIQUID FCC
  11 ALF  < unused >  1548.0      LIQUID FCC
  12 ALF  < unused >  1499.0      LIQUID FCC
  13 ALF  < unused >  1438.0      LIQUID FCC
  20 ATIE   3   1.    1413.0      LIQUID FCC
  21 ATIE   3   1.    1337.0      LIQUID FCC
  22 ATIE   3   1.    1213.0      LIQUID FCC
  23 ATIE   3   1.    1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     2   1.    1773.0      LIQUID
 116 AH     2   1.    1773.0      LIQUID
 117 AH     2   1.    1773.0      LIQUID
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
ED_EXP: @@ any liquid parameters and restore those with label ALF
ED_EXP: s-we 0 100-118
   ... the command in full is SET_WEIGHT
ED_EXP: s-we 1 alf
   ... the command in full is SET_WEIGHT
 Changed weight on                        4  equilibria.
ED_EXP: s-e 1
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                        1 , label AINV
ED_EXP: c-a
```

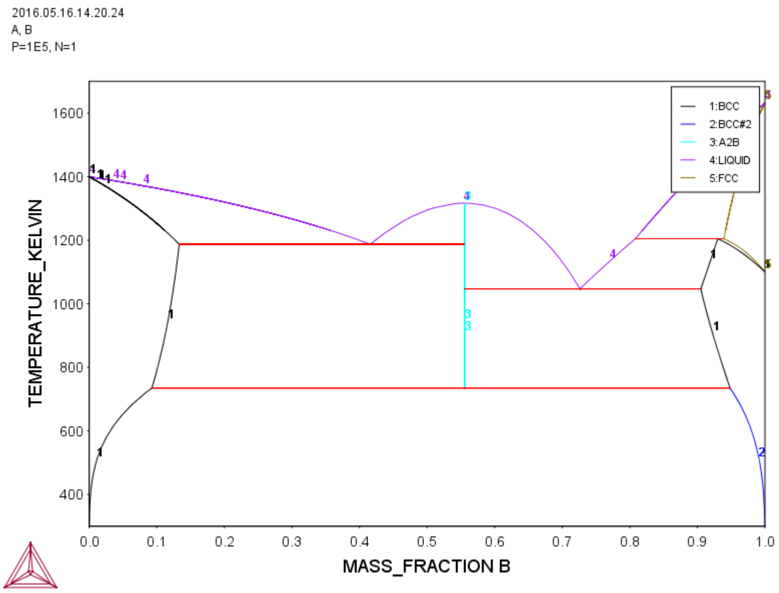
```
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1187.5      LIQUID A2B BCC
   2 AINV   2   1.    1316.7      LIQUID A2B
   3 AINV   2   1.    1047.0      LIQUID A2B BCC
   4 AINV   2   1.    1204.7      LIQUID BCC FCC
   5 AINV   2   1.     734.7      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    6   1.    1594.0      LIQUID FCC
  11 ALF    6   1.    1548.0      LIQUID FCC
  12 ALF    7   1.    1499.0      LIQUID FCC
  13 ALF    7   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA   < unused >  1573.0      LIQUID
 101 AA   < unused >  1573.0      LIQUID
 102 AA   < unused >  1573.0      LIQUID
 103 AA   < unused >  1573.0      LIQUID
 104 AA   < unused >  1573.0      LIQUID
 105 AA   < unused >  1573.0      LIQUID
 106 AA   < unused >  1573.0      LIQUID
 107 AA   < unused >  1573.0      LIQUID
 108 AA   < unused >  1573.0      LIQUID
 110 AH   < unused >  1773.0      LIQUID
 111 AH   < unused >  1773.0      LIQUID
 112 AH   < unused >  1773.0      LIQUID
 113 AH   < unused >  1773.0      LIQUID
 114 AH   < unused >  1773.0      LIQUID
 115 AH   < unused >  1773.0      LIQUID
 116 AH   < unused >  1773.0      LIQUID
 117 AH   < unused >  1773.0      LIQUID
 118 AH   < unused >  1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20:20




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02757864E+04    2.02757864E+04    2.02757864E+04    7.39333291E-02
 V2     -2.90134088E+01   -2.90134088E+01   -2.90134088E+01    3.44753302E-01
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     2.39869483E+04    2.39869483E+04    2.39869483E+04    6.19220768E-01
 V16    -8.02178633E+00   -8.02178633E+00   -8.02178633E+00    2.18789658E+00
 V17     3.13540526E+03    3.13540526E+03    3.13540526E+03    1.44882543E+00
 V19     2.12643554E+04    2.12643554E+04    2.12643554E+04    4.78622311E+00
 V20    -6.23643289E+00   -6.23643289E+00   -6.23643289E+00    1.26469088E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   3.83968704E-01 TO   7.41792272E+00
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   3.37178306E-01



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1187.      10.0      -5.532     -0.5532
1 W(LIQUID,B)=0.408              0.4157      2.00E-02  7.7215E-03  0.3861
1 W(BCC,B)=0.13                  0.1332      2.00E-02  3.2119E-03  0.1606
2 T=1341                          1317.      10.0      -24.32      -2.432
2 HTR=3727                        3727.      5.00E+02  0.4611      9.2229E-04
3 T=1049                          1047.      10.0      -1.990     -0.1990
3 W(LIQUID,A)=0.27               0.2739      2.00E-02  3.9062E-03  0.1953
3 W(BCC,A)=9.3E-2                9.4971E-02  2.00E-02  1.9713E-03  9.8563E-02
4 T=1203                          1205.      10.0       1.671      0.1671
4 W(LIQUID,A)=0.19               0.1919      2.00E-02  1.8666E-03  9.3330E-02
4 W(BCC,A)=6.9E-2                6.9780E-02  2.00E-02  7.8014E-04  3.9007E-02
4 W(FCC,A)=6E-2                  6.0794E-02  2.00E-02  7.9445E-04  3.9723E-02
5 T=726                           734.7      10.0       8.703      0.8703
5 X(BCC,B)=3.7E-2                3.9289E-02  2.00E-02  2.2886E-03  0.1144
5 X(BCC#2,A)=0.114               0.1200      2.00E-02  6.0001E-03  0.3000
6 X(BCC,B)=3.7E-2                3.6833E-02  2.00E-02 -1.6665E-04 -8.3327E-03
6 X(BCC#2,A)=0.114               0.1140      2.00E-02 -1.6829E-05 -8.4144E-04
10 W(LIQUID,A)=2E-2              1.9506E-02  2.00E-02 -4.9427E-04 -2.4713E-02
```

```
11 W(LIQUID,A)=4.2E-2            4.1827E-02  2.00E-02 -1.7330E-04 -8.6648E-03
12 W(LIQUID,A)=6.5E-2            6.5040E-02  2.00E-02  4.0133E-05  2.0066E-03
13 W(LIQUID,A)=9.3E-2            9.3114E-02  2.00E-02  1.1416E-04  5.7082E-03
20 W(LIQUID,A)=0.104             0.1043      2.00E-02  3.4980E-04  1.7490E-02
20 W(FCC,A)=3.8E-2               3.8244E-02  2.00E-02  2.4396E-04  1.2198E-02
21 W(LIQUID,A)=0.136             0.1375      2.00E-02  1.5284E-03  7.6418E-02
21 W(FCC,A)=4.7E-2               4.7395E-02  2.00E-02  3.9496E-04  1.9748E-02
22 W(LIQUID,A)=0.187             0.1886      2.00E-02  1.5692E-03  7.8460E-02
22 W(FCC,A)=5.9E-2               6.0019E-02  2.00E-02  1.0194E-03  5.0968E-02
23 W(LIQUID,A)=0.245             0.2474      2.00E-02  2.3699E-03  0.1185
23 W(BCC,A)=8.5E-2               8.6337E-02  2.00E-02  1.3367E-03  6.6834E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for equilibrium 4
PARROT: @@ It can be on the wrong side, at high A instead of high B. Try to correct
PARROT: @@ that in the edit module.
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                      4 , label AINV
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.671469/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /*/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database: UNKNOWN

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC=1     FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1204.67 K (   931.52 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.29910E+02
 Total Gibbs energy -9.73780E+03,  Enthalpy  1.97627E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.6968E-01  1.0310E-01 4.0116E-01 -9.1489E+03 SER
 B                       2.3303E+00  8.9690E-01 8.5667E-01 -1.5496E+03 SER

 FCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5821E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.39206E-01  A  6.07945E-02

 BCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5262E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.30220E-01  A  6.97801E-02

 LIQUID                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.8826E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.08133E-01  A  1.91867E-01

 EXPERIMENT T=1203:DT  $1204.67:10  NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX  $0.191867:2E-2  NO=2
 EXPERIMENT W(BCC,A)=6.9E-2:DX  $6.97801E-2:2E-2  NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX  $6.07945E-2:2E-2  NO=4
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ The error is still there, calculate the phase diagram!!!
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
```

```
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC
  ** BCC#2
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC
  ** BCC#2
 Calculated.                     14  equilibria

 Phase region boundary   3 at:   6.802E-01  7.347E+02
  ** A2B
     BCC
  ** BCC#2

 Phase region boundary   4 at:   3.640E-01  7.347E+02
  ** A2B
     BCC
 Calculated.                     14  equilibria

 Phase region boundary   5 at:   3.781E-01  1.187E+03
  ** LIQUID
  ** A2B
     BCC

 Phase region boundary   6 at:   2.888E-01  1.187E+03
  ** LIQUID
     BCC
 Calculated                     27  equilibria

 Phase region boundary   7 at:   4.898E-01  1.187E+03
  ** LIQUID
     A2B
 Calculated.                     26  equilibria

 Phase region boundary   8 at:   6.479E-01  1.047E+03
  ** LIQUID
     A2B
  ** BCC

 Phase region boundary   9 at:   7.629E-01  1.047E+03
     A2B
  ** BCC
 Calculated.                     10  equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   8.250E-01  1.047E+03
     LIQUID
  ** BCC
 Calculated.                      9  equilibria
```

```
Phase region boundary  11 at:   8.738E-01  1.205E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.791E-01  1.205E+03
    LIQUID
 ** FCC
Calculated                     37  equilibria

Phase region boundary  13 at:   9.347E-01  1.205E+03
    BCC
 ** FCC
Calculated                     26  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.657E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  26 at:   3.657E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.657E-01  7.700E+02
 ** A2B
    BCC
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.900E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  29 at:   7.900E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.900E-01  7.700E+02
```

```
  ** A2B
     BCC
 Calculated.                      9  equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.459E-01  1.230E+03
  ** LIQUID
     BCC
 Calculated.                      4  equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.459E-01  1.230E+03
  ** LIQUID
     BCC
 Calculated                     26  equilibria

 Phase region boundary  33 at:   8.847E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                      2  equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.847E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                     29  equilibria

 Phase region boundary  35 at:   6.422E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated                      9  equilibria

 Phase region boundary  36 at:   6.422E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated.                     13  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC
 Calculated                     19  equilibria

 Phase region boundary  38 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC
 Calculated.                      4  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.219E+03
     LIQUID
  ** A2B
 Calculated.                     12  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.219E+03
     LIQUID
  ** A2B
 Calculated.                      7  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                     20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                     13  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                      0  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: s-we 0 4
   ... the command in full is SET_WEIGHT
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use       25 experiments, maximum is        2000
 Use      494 real workspace, maximum is    50000
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20:24



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =    0    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02757864E+04    2.02757864E+04    2.02757864E+04    7.39333291E-02
 V2     -2.90134088E+01   -2.90134088E+01   -2.90134088E+01    3.44753302E-01
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     2.39869483E+04    2.39869483E+04    2.39869483E+04    6.19220768E-01
 V16    -8.02178633E+00   -8.02178633E+00   -8.02178633E+00    2.18789658E+00
 V17     3.13540526E+03    3.13540526E+03    3.13540526E+03    1.44882543E+00
 V19     2.12643554E+04    2.12643554E+04    2.12643554E+04    4.78622311E+00
 V20    -6.23643289E+00   -6.23643289E+00   -6.23643289E+00    1.26469088E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   3.83968704E-01 TO   7.37817472E+00
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   4.09898596E-01


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
```

```
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1187.      10.0      -5.532     -0.5532
1 W(LIQUID,B)=0.408              0.4157     2.00E-02  7.7215E-03  0.3861
1 W(BCC,B)=0.13                  0.1332     2.00E-02  3.2119E-03  0.1606
2 T=1341                          1317.      10.0      -24.32      -2.432
2 HTR=3727                        3727.     5.00E+02  0.4611      9.2229E-04
3 T=1049                          1047.      10.0      -1.990     -0.1990
3 W(LIQUID,A)=0.27               0.2739     2.00E-02  3.9062E-03  0.1953
3 W(BCC,A)=9.3E-2                9.4971E-02 2.00E-02  1.9713E-03  9.8563E-02
5 T=726                           734.7      10.0       8.703      0.8703
5 X(BCC,B)=3.7E-2                3.9289E-02 2.00E-02  2.2886E-03  0.1144
5 X(BCC#2,A)=0.114               0.1200     2.00E-02  6.0001E-03  0.3000
6 X(BCC,B)=3.7E-2                3.6833E-02 2.00E-02 -1.6665E-04 -8.3327E-03
6 X(BCC#2,A)=0.114               0.1140     2.00E-02 -1.6829E-05 -8.4144E-04
10 W(LIQUID,A)=2E-2              1.9506E-02 2.00E-02 -4.9427E-04 -2.4713E-02
11 W(LIQUID,A)=4.2E-2            4.1827E-02 2.00E-02 -1.7330E-04 -8.6648E-03
12 W(LIQUID,A)=6.5E-2            6.5040E-02 2.00E-02  4.0133E-05  2.0066E-03
13 W(LIQUID,A)=9.3E-2            9.3114E-02 2.00E-02  1.1416E-04  5.7082E-03
20 W(LIQUID,A)=0.104             0.1043     2.00E-02  3.4980E-04  1.7490E-02
20 W(FCC,A)=3.8E-2               3.8244E-02 2.00E-02  2.4396E-04  1.2198E-02
21 W(LIQUID,A)=0.136             0.1375     2.00E-02  1.5284E-03  7.6418E-02
21 W(FCC,A)=4.7E-2               4.7395E-02 2.00E-02  3.9496E-04  1.9748E-02
22 W(LIQUID,A)=0.187             0.1886     2.00E-02  1.5692E-03  7.8460E-02
22 W(FCC,A)=5.9E-2               6.0019E-02 2.00E-02  1.0194E-03  5.0968E-02
23 W(LIQUID,A)=0.245             0.2474     2.00E-02  2.3699E-03  0.1185
23 W(BCC,A)=8.5E-2               8.6337E-02 2.00E-02  1.3367E-03  6.6834E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use       25 experiments, maximum is        2000
 Use      494 real workspace, maximum is     50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    7.37817472E+00
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    7.53019237E+00
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    7.11518144E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    7.10968662E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    7.11099046E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    7.10983084E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    7.10931183E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    7.10944990E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    3.63987301E-01
  1  9.9778E-01   2  1.0040E+00   3  1.0002E+00   4  9.9998E-01   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    3.27827938E-01
  1  9.9774E-01   2  1.0037E+00   3  1.0002E+00   4  9.9757E-01   5  9.9826E-01
  6  1.0015E+00   7  1.0030E+00

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    2.68447716E-01
  1  9.9735E-01   2  1.0038E+00   3  9.9865E-01   4  9.9067E-01   5  9.9310E-01
  6  1.0027E+00   7  1.0046E+00

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    2.16955159E-01
  1  9.9691E-01   2  1.0034E+00   3  9.9639E-01   4  9.8058E-01   5  9.8548E-01
  6  1.0080E+00   7  1.0160E+00

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.51367607E-01
  1  9.9564E-01   2  1.0029E+00   3  9.8912E-01   4  9.5293E-01   5  9.6407E-01
  6  1.0089E+00   7  1.0123E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   12 iterations
  1  9.9564E-01   2  1.0029E+00   3  9.8912E-01   4  9.5293E-01   5  9.6407E-01
  6  1.0089E+00   7  1.0123E+00

  1  7.0458E-02   2 -3.9714E-02   3 -7.7917E-02   4 -7.3557E-02   5  5.9818E-02
  6  2.5625E-01   7 -1.8711E-02   8 -9.5448E-02   9  1.6592E-01  10  5.4874E-02
 11 -3.7948E-02  12  3.1686E-02  13 -9.3446E-02  14 -2.8663E-02  15 -1.6943E-02
 16 -1.0570E-02  17 -1.1807E-02  18 -1.9285E-03  19 -9.4044E-03  20  5.1591E-02
 21 -1.0495E-02  22  4.5740E-02  23  2.4209E-03  24  1.2336E-02  25 -8.0309E-02

               THE SUM OF SQUARES IS   1.51367607E-01
PARROT: cont 30
   ... the command in full is CONTINUE_OPTIMIZATION

 It is safe to CONTINUE only after TOO MANY ITERATIONS
 and no change in variables and experiments ...
 Now anything can happen ...

PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


          ===================================================
          OUTPUT FROM   P A R R O T.  DATE 2016. 5.16   14:20:24
```

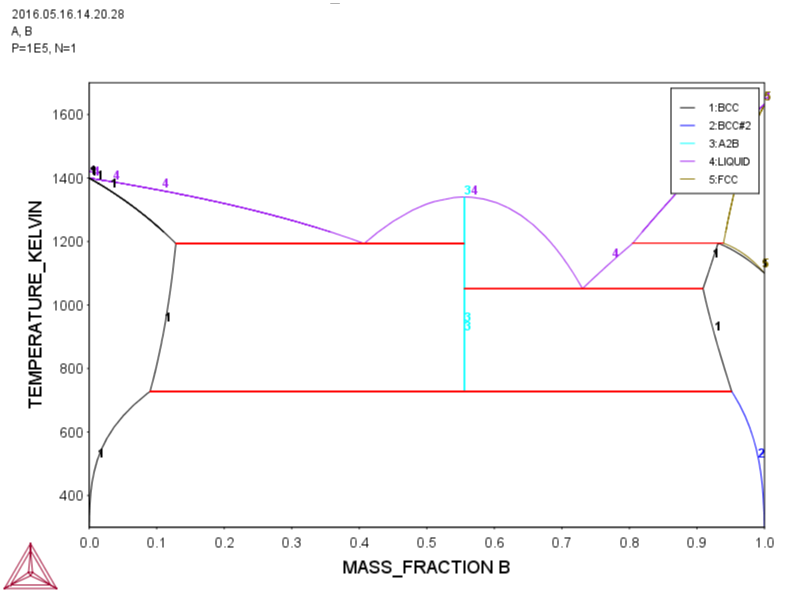
```
 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  13


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.01874435E+04    2.02757864E+04    2.02757864E+04    2.69317159E-02
 V2     -2.90969417E+01   -2.90134088E+01   -2.90134088E+01    1.50772675E-02
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     2.37258616E+04    2.39869483E+04    2.39869483E+04    9.90009036E-02
 V16    -7.64416251E+00   -8.02178633E+00   -8.02178633E+00    3.01534612E-01
 V17     3.02274705E+03    3.13540526E+03    3.13540526E+03    2.49736435E-01
 V19     2.14533478E+04    2.12643554E+04    2.12643554E+04    6.60453317E-01
 V20    -6.31327793E+00   -6.23643289E+00   -6.23643289E+00    1.71543397E+00

 NUMBER OF OPTIMIZING VARIABLES :    7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM    7.37817472E+00 TO    1.51367607E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.40931149E-03



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.      10.0      0.7046      7.0458E-02
1 W(LIQUID,B)=0.408              0.4072      2.00E-02 -7.9429E-04 -3.9714E-02
1 W(BCC,B)=0.13                  0.1284      2.00E-02 -1.5583E-03 -7.7917E-02
2 T=1341                          1340.      10.0     -0.7356     -7.3557E-02
2 HTR=3727                        3757.      5.00E+02   29.91      5.9818E-02
3 T=1049                          1052.      10.0       2.563      0.2563
3 W(LIQUID,A)=0.27               0.2696      2.00E-02 -3.7422E-04 -1.8711E-02
3 W(BCC,A)=9.3E-2                9.1091E-02  2.00E-02 -1.9090E-03 -9.5448E-02
5 T=726                           727.7      10.0       1.659      0.1659
5 X(BCC,B)=3.7E-2                3.8097E-02  2.00E-02  1.0975E-03  5.4874E-02
5 X(BCC#2,A)=0.114               0.1132      2.00E-02 -7.5897E-04 -3.7948E-02
6 X(BCC,B)=3.7E-2                3.7634E-02  2.00E-02  6.3372E-04  3.1686E-02
6 X(BCC#2,A)=0.114               0.1121      2.00E-02 -1.8689E-03 -9.3446E-02
10 W(LIQUID,A)=2E-2              1.9427E-02  2.00E-02 -5.7326E-04 -2.8663E-02
11 W(LIQUID,A)=4.2E-2            4.1661E-02  2.00E-02 -3.3885E-04 -1.6943E-02
12 W(LIQUID,A)=6.5E-2            6.4789E-02  2.00E-02 -2.1139E-04 -1.0570E-02
13 W(LIQUID,A)=9.3E-2            9.2764E-02  2.00E-02 -2.3614E-04 -1.1807E-02
20 W(LIQUID,A)=0.104             0.1040      2.00E-02 -3.8571E-05 -1.9285E-03
20 W(FCC,A)=3.8E-2               3.7812E-02  2.00E-02 -1.8809E-04 -9.4044E-03
21 W(LIQUID,A)=0.136             0.1370      2.00E-02  1.0318E-03  5.1591E-02
21 W(FCC,A)=4.7E-2               4.6790E-02  2.00E-02 -2.0989E-04 -1.0495E-02
22 W(LIQUID,A)=0.187             0.1879      2.00E-02  9.1479E-04  4.5740E-02
22 W(FCC,A)=5.9E-2               5.9048E-02  2.00E-02  4.8418E-05  2.4209E-03
23 W(LIQUID,A)=0.245             0.2452      2.00E-02  2.4672E-04  1.2336E-02
23 W(BCC,A)=8.5E-2               8.3394E-02  2.00E-02 -1.6062E-03 -8.0309E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Optimization converged, try to add equilibrium 4 again
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                       4 , label AINV
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.671469/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC=1      FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1194.80 K (   921.65 C),  Pressure  1.013250E+05
```

```
 Number of moles of components  3.00000E+00,  Mass in grams  1.29837E+02
 Total Gibbs energy -9.46749E+03,  Enthalpy  1.96784E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.7209E-01  1.0353E-01 4.0897E-01 -8.8824E+03 SER
 B                       2.3279E+00  8.9647E-01 8.5964E-01 -1.5025E+03 SER

 FCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5830E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.39335E-01  A  6.06655E-02

 BCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5327E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.31263E-01  A  6.87372E-02

 LIQUID                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.8681E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.04923E-01  A  1.95077E-01

 SET_WEIGHT 0,,,
 EXPERIMENT T=1203:DT
 EXPERIMENT W(LIQUID,A)=0.19:DX
 EXPERIMENT W(BCC,A)=6.9E-2:DX
 EXPERIMENT W(FCC,A)=6E-2:DX
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
```

```
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28

Phase region boundary   1 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary   2 at:   7.141E-01  3.000E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria

Phase region boundary   3 at:   6.826E-01  7.277E+02
 ** A2B
    BCC
 ** BCC#2

Phase region boundary   4 at:   3.631E-01  7.277E+02
 ** A2B
    BCC
Calculated.                     15  equilibria

Phase region boundary   5 at:   3.764E-01  1.194E+03
 ** LIQUID
 ** A2B
    BCC

Phase region boundary   6 at:   2.817E-01  1.194E+03
 ** LIQUID
    BCC
Calculated                     24  equilibria

Phase region boundary   7 at:   4.860E-01  1.194E+03
 ** LIQUID
    A2B
Calculated.                     28  equilibria

Phase region boundary   8 at:   6.504E-01  1.052E+03
 ** LIQUID
    A2B
 ** BCC

Phase region boundary   9 at:   7.656E-01  1.052E+03
    A2B
 ** BCC
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.290E-01  1.052E+03
    LIQUID
 ** BCC
Calculated.                      8  equilibria

Phase region boundary  11 at:   8.731E-01  1.195E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.778E-01  1.195E+03
    LIQUID
 ** FCC
Calculated                     36  equilibria

Phase region boundary  13 at:   9.353E-01  1.195E+03
    BCC
 ** FCC
Calculated                     21  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
```

```
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.649E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  26 at:   3.649E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.649E-01  7.700E+02
 ** A2B
    BCC
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.918E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  29 at:   7.918E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.918E-01  7.700E+02
 ** A2B
    BCC
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.447E-01  1.230E+03
 ** LIQUID
    BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.447E-01  1.230E+03
 ** LIQUID
    BCC
Calculated                     26  equilibria

Phase region boundary  33 at:   8.855E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.855E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                     29  equilibria

Phase region boundary  35 at:   6.403E-03  1.397E+03
    LIQUID
 ** BCC
Calculated                      9  equilibria

Phase region boundary  36 at:   6.403E-03  1.397E+03
    LIQUID
 ** BCC
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.294E-01  1.244E+03
    LIQUID
 ** BCC
Calculated                     21  equilibria

Phase region boundary  38 at:   2.294E-01  1.244E+03
    LIQUID
 ** BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.242E+03
    LIQUID
 ** A2B
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.122E-01  1.242E+03
```

```
     LIQUID
  ** A2B
 Calculated.                      8  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                     20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                     13  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                     1  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ Sometimes a very strange shape of the fcc phase here and no
POST: @@ equilibrium between liq, fcc and bcc at high B content.
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20:28




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  13


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.01874435E+04    2.02757864E+04    2.02757864E+04    2.69317159E-02
 V2     -2.90969417E+01   -2.90134088E+01   -2.90134088E+01    1.50772675E-02
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     2.37258616E+04    2.39869483E+04    2.39869483E+04    9.90009036E-02
 V16    -7.64416251E+00   -8.02178633E+00   -8.02178633E+00    3.01534612E-01
```

```
 V17     3.02274705E+03    3.13540526E+03    3.13540526E+03    2.49736435E-01
 V19     2.14533478E+04    2.12643554E+04    2.12643554E+04    6.60453317E-01
 V20    -6.31327793E+00   -6.23643289E+00   -6.23643289E+00    1.71543397E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   7.37817472E+00 TO   1.51367607E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.40931149E-03



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.      10.0      0.7046      7.0458E-02
1 W(LIQUID,B)=0.408              0.4072      2.00E-02 -7.9429E-04 -3.9714E-02
1 W(BCC,B)=0.13                  0.1284      2.00E-02 -1.5583E-03 -7.7917E-02
2 T=1341                          1340.      10.0     -0.7356     -7.3557E-02
2 HTR=3727                        3757.      5.00E+02   29.91      5.9818E-02
3 T=1049                          1052.      10.0       2.563      0.2563
3 W(LIQUID,A)=0.27               0.2696      2.00E-02 -3.7422E-04 -1.8711E-02
3 W(BCC,A)=9.3E-2                9.1091E-02  2.00E-02 -1.9090E-03 -9.5448E-02
5 T=726                           727.7      10.0       1.659      0.1659
5 X(BCC,B)=3.7E-2                3.8097E-02  2.00E-02  1.0975E-03  5.4874E-02
5 X(BCC#2,A)=0.114               0.1132      2.00E-02 -7.5897E-04 -3.7948E-02
6 X(BCC,B)=3.7E-2                3.7634E-02  2.00E-02  6.3372E-04  3.1686E-02
6 X(BCC#2,A)=0.114               0.1121      2.00E-02 -1.8689E-03 -9.3446E-02
10 W(LIQUID,A)=2E-2              1.9427E-02  2.00E-02 -5.7326E-04 -2.8663E-02
11 W(LIQUID,A)=4.2E-2            4.1661E-02  2.00E-02 -3.3885E-04 -1.6943E-02
12 W(LIQUID,A)=6.5E-2            6.4789E-02  2.00E-02 -2.1139E-04 -1.0570E-02
13 W(LIQUID,A)=9.3E-2            9.2764E-02  2.00E-02 -2.3614E-04 -1.1807E-02
20 W(LIQUID,A)=0.104             0.1040      2.00E-02 -3.8571E-05 -1.9285E-03
20 W(FCC,A)=3.8E-2               3.7812E-02  2.00E-02 -1.8809E-04 -9.4044E-03
21 W(LIQUID,A)=0.136             0.1370      2.00E-02  1.0318E-03  5.1591E-02
21 W(FCC,A)=4.7E-2               4.6790E-02  2.00E-02 -2.0989E-04 -1.0495E-02
22 W(LIQUID,A)=0.187             0.1879      2.00E-02  9.1479E-04  4.5740E-02
22 W(FCC,A)=5.9E-2               5.9048E-02  2.00E-02  4.8418E-05  2.4209E-03
23 W(LIQUID,A)=0.245             0.2452      2.00E-02  2.4672E-04  1.2336E-02
23 W(BCC,A)=8.5E-2               8.3394E-02  2.00E-02 -1.6062E-03 -8.0309E-02


PARROT:
PARROT: @@ Note that all other experiments are well fitted!
PARROT: @@ Try to improve by optimizing a little more !!!
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use      25 experiments, maximum is       2000
 Use     494 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    1.51367607E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    1.52533051E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    1.53440354E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.50571317E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50814099E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50610770E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50503265E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50524533E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50302078E-01
  1  9.9999E-01   2  1.0000E+00   3  1.0001E+00   4  9.9998E-01   5  9.9999E-01
  6  1.0001E+00   7  1.0001E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50110907E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  9.9996E-01   5  9.9998E-01
  6  1.0002E+00   7  1.0002E+00

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49917194E-01
  1  9.9999E-01   2  1.0000E+00   3  1.0002E+00   4  9.9992E-01   5  9.9996E-01
  6  1.0002E+00   7  1.0003E+00

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49701897E-01
  1  9.9999E-01   2  1.0000E+00   3  1.0002E+00   4  9.9986E-01   5  9.9992E-01
  6  1.0004E+00   7  1.0007E+00

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49443230E-01
  1  9.9998E-01   2  1.0000E+00   3  1.0002E+00   4  9.9974E-01   5  9.9985E-01
  6  1.0007E+00   7  1.0014E+00

      AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49088139E-01
  1  9.9998E-01   2  1.0000E+00   3  1.0001E+00   4  9.9950E-01   5  9.9971E-01
  6  1.0013E+00   7  1.0029E+00

      AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48551477E-01
  1  9.9996E-01   2  1.0000E+00   3  1.0000E+00   4  9.9904E-01   5  9.9942E-01
  6  1.0024E+00   7  1.0058E+00
```

```
      AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49192907E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  9.9904E-01   5  9.9942E-01
  6  1.0025E+00   7  1.0058E+00

      AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50825500E-01
  1  9.9998E-01   2  1.0001E+00   3  1.0000E+00   4  9.9903E-01   5  9.9942E-01
  6  1.0024E+00   7  1.0058E+00

      AT THE   17 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48149051E-01
  1  9.9998E-01   2  9.9998E-01   3  1.0001E+00   4  9.9903E-01   5  9.9942E-01
  6  1.0024E+00   7  1.0058E+00

      AT THE   18 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48106327E-01
  1  9.9997E-01   2  1.0000E+00   3  1.0001E+00   4  9.9912E-01   5  9.9942E-01
  6  1.0024E+00   7  1.0059E+00

      AT THE   19 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48103802E-01
  1  9.9996E-01   2  1.0000E+00   3  1.0001E+00   4  9.9912E-01   5  9.9951E-01
  6  1.0025E+00   7  1.0059E+00

      AT THE   20 TH ITERATION WE HAVE THE SUM OF SQUARES    1.47348969E-01
  1  9.9995E-01   2  9.9998E-01   3  9.9990E-01   4  9.9819E-01   5  9.9893E-01
  6  1.0048E+00   7  1.0117E+00

      AT THE   21 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48042770E-01
  1  9.9997E-01   2  9.9996E-01   3  9.9986E-01   4  9.9823E-01   5  9.9895E-01
  6  1.0047E+00   7  1.0117E+00

      AT THE   22 TH ITERATION WE HAVE THE SUM OF SQUARES    1.46175461E-01
  1  9.9990E-01   2  9.9997E-01   3  9.9943E-01   4  9.9635E-01   5  9.9778E-01
  6  1.0094E+00   7  1.0234E+00

      AT THE   23 TH ITERATION WE HAVE THE SUM OF SQUARES    1.44759679E-01
  1  9.9981E-01   2  9.9992E-01   3  9.9844E-01   4  9.9265E-01   5  9.9546E-01
  6  1.0188E+00   7  1.0468E+00

      AT THE   24 TH ITERATION WE HAVE THE SUM OF SQUARES    1.44427075E-01
  1  9.9973E-01   2  9.9989E-01   3  9.9765E-01   4  9.8970E-01   5  9.9361E-01
  6  1.0261E+00   7  1.0652E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   24 iterations
  1  9.9973E-01   2  9.9989E-01   3  9.9765E-01   4  9.8970E-01   5  9.9361E-01
  6  1.0261E+00   7  1.0652E+00

  1  6.6807E-02   2 -4.4958E-02   3 -9.7560E-02   4 -6.3010E-02   5  6.3385E-02
  6  2.1373E-01   7 -2.7115E-02   8 -1.2155E-01   9  1.5013E-01  10  5.9941E-02
 11 -5.8436E-02  12  3.8935E-02  13 -1.0845E-01  14 -2.2928E-02  15 -7.7951E-03
 16 -8.4310E-04  17 -4.6848E-03  18  3.2982E-03  19 -3.5905E-03  20  4.8873E-02
 21 -1.3805E-02  22  2.5374E-02  23 -2.7745E-02  24 -7.5343E-03  25 -1.0836E-01

               THE SUM OF SQUARES IS   1.44427075E-01
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


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           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20:28




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  25


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.01820918E+04    2.01874435E+04    2.01874435E+04    2.60519708E-02
 V2     -2.90936108E+01   -2.90969417E+01   -2.90969417E+01    1.41576502E-02
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     2.36701045E+04    2.37258616E+04    2.37258616E+04    1.00528943E-01
 V16    -7.56540324E+00   -7.64416251E+00   -7.64416251E+00    3.17219075E-01
 V17     3.00342248E+03    3.02274705E+03    3.02274705E+03    2.60675642E-01
 V19     2.20133196E+04    2.14533478E+04    2.14533478E+04    6.92926768E-01
 V20    -6.72497818E+00   -6.31327793E+00   -6.31327793E+00    1.79244330E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.51367607E-01 TO   1.44427075E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.02372640E-03



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.      10.0      0.6681      6.6807E-02
1 W(LIQUID,B)=0.408              0.4071      2.00E-02 -8.9916E-04 -4.4958E-02
1 W(BCC,B)=0.13                  0.1280      2.00E-02 -1.9512E-03 -9.7560E-02
2 T=1341                          1340.      10.0     -0.6301     -6.3010E-02
2 HTR=3727                        3759.      5.00E+02   31.69      6.3385E-02
3 T=1049                          1051.      10.0       2.137      0.2137
3 W(LIQUID,A)=0.27               0.2695      2.00E-02 -5.4230E-04 -2.7115E-02
3 W(BCC,A)=9.3E-2                9.0569E-02  2.00E-02 -2.4311E-03 -0.1216
5 T=726                           727.5      10.0       1.501      0.1501
5 X(BCC,B)=3.7E-2                3.8199E-02  2.00E-02  1.1988E-03  5.9941E-02
```
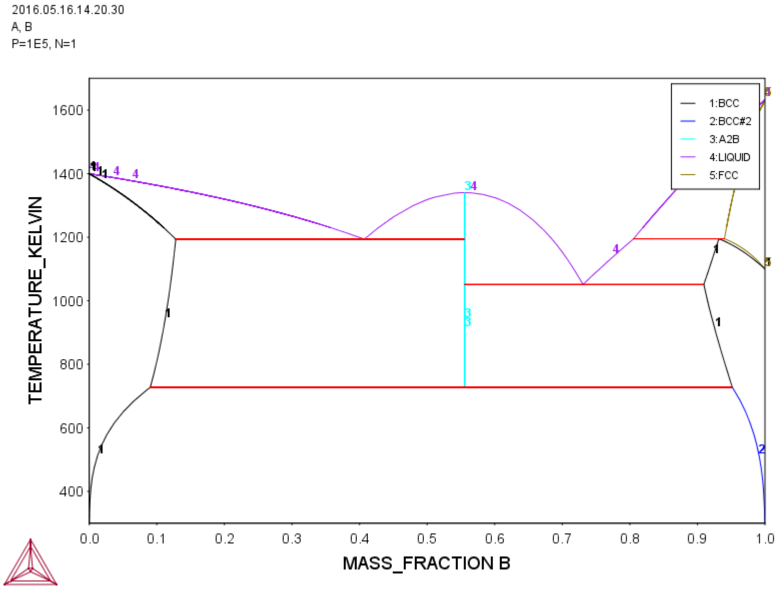

```
5 X(BCC#2,A)=0.114               0.1128      2.00E-02 -1.1687E-03 -5.8436E-02
6 X(BCC,B)=3.7E-2                3.7779E-02  2.00E-02  7.7870E-04  3.8935E-02
6 X(BCC#2,A)=0.114               0.1118      2.00E-02 -2.1691E-03 -0.1085
10 W(LIQUID,A)=2E-2              1.9541E-02  2.00E-02 -4.5856E-04 -2.2928E-02
11 W(LIQUID,A)=4.2E-2            4.1844E-02  2.00E-02 -1.5590E-04 -7.7951E-03
12 W(LIQUID,A)=6.5E-2            6.4983E-02  2.00E-02 -1.6862E-05 -8.4310E-04
13 W(LIQUID,A)=9.3E-2            9.2906E-02  2.00E-02 -9.3697E-05 -4.6848E-03
20 W(LIQUID,A)=0.104             0.1041      2.00E-02  6.5965E-05  3.2982E-03
20 W(FCC,A)=3.8E-2               3.7928E-02  2.00E-02 -7.1810E-05 -3.5905E-03
21 W(LIQUID,A)=0.136             0.1370      2.00E-02  9.7746E-04  4.8873E-02
21 W(FCC,A)=4.7E-2               4.6724E-02  2.00E-02 -2.7609E-04 -1.3805E-02
22 W(LIQUID,A)=0.187             0.1875      2.00E-02  5.0747E-04  2.5374E-02
22 W(FCC,A)=5.9E-2               5.8445E-02  2.00E-02 -5.5491E-04 -2.7745E-02
23 W(LIQUID,A)=0.245             0.2448      2.00E-02 -1.5069E-04 -7.5343E-03
23 W(BCC,A)=8.5E-2               8.2833E-02  2.00E-02 -2.1672E-03 -0.1084


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram again
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
```

```
Generating start point  28

Phase region boundary   1 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary   2 at:   7.141E-01  3.000E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria

Phase region boundary   3 at:   6.828E-01  7.275E+02
 ** A2B
    BCC
 ** BCC#2

Phase region boundary   4 at:   3.632E-01  7.275E+02
 ** A2B
    BCC
Calculated.                     15  equilibria

Phase region boundary   5 at:   3.763E-01  1.194E+03
 ** LIQUID
 ** A2B
    BCC

Phase region boundary   6 at:   2.815E-01  1.194E+03
 ** LIQUID
    BCC
Calculated                     27  equilibria

Phase region boundary   7 at:   4.860E-01  1.194E+03
 ** LIQUID
    A2B
Calculated.                     28  equilibria

Phase region boundary   8 at:   6.505E-01  1.051E+03
 ** LIQUID
    A2B
 ** BCC

Phase region boundary   9 at:   7.660E-01  1.051E+03
    A2B
 ** BCC
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.294E-01  1.051E+03
    LIQUID
 ** BCC
Calculated.                      8  equilibria

Phase region boundary  11 at:   8.737E-01  1.195E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.785E-01  1.195E+03
    LIQUID
 ** FCC
Calculated                     31  equilibria

Phase region boundary  13 at:   9.360E-01  1.195E+03
    BCC
 ** FCC
Calculated                     27  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
```

```
    BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.650E-01  7.700E+02
 ** A2B
    BCC
Calculated                      10  equilibria

Phase region boundary  26 at:   3.650E-01  7.700E+02
 ** A2B
    BCC
Calculated.                       3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.650E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      14  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.919E-01  7.700E+02
 ** A2B
    BCC
Calculated                      10  equilibria

Phase region boundary  29 at:   7.919E-01  7.700E+02
 ** A2B
    BCC
Calculated.                       3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.919E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      10  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.445E-01  1.230E+03
 ** LIQUID
    BCC
Calculated.                       4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.445E-01  1.230E+03
 ** LIQUID
    BCC
Calculated                      26  equilibria

Phase region boundary  33 at:   8.860E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                       2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.860E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                      29  equilibria

Phase region boundary  35 at:   6.399E-03  1.397E+03
    LIQUID
 ** BCC
Calculated                      10  equilibria

Phase region boundary  36 at:   6.399E-03  1.397E+03
    LIQUID
 ** BCC
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.293E-01  1.244E+03
    LIQUID
 ** BCC
Calculated                      21  equilibria

Phase region boundary  38 at:   2.293E-01  1.244E+03
    LIQUID
 ** BCC
Calculated.                       4  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.242E+03
    LIQUID
 ** A2B
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.122E-01  1.242E+03
    LIQUID
 ** A2B
Calculated.                       8  equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   9.927E-01  1.613E+03
    LIQUID
```

```
  ** FCC
 Calculated.                      20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      12  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                      1  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid at high B
PARROT: @@ restore equilibrium 4 on the POP file
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                      4 , label AINV
ED_EXP: s-we 1
   ... the command in full is SET_WEIGHT
Equilibria (range) or label(s) /PRESENT/: PRESENT
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.671469/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC=1     FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1195.10 K (   921.95 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.29944E+02
 Total Gibbs energy -9.43346E+03,  Enthalpy  1.97100E+04,  Volume  0.00000E+00
```

```
 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.6854E-01  1.0290E-01 4.0783E-01 -8.9123E+03 SER
 B                       2.3315E+00  8.9710E-01 8.6070E-01 -1.4906E+03 SER

 FCC                          Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5876E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.40072E-01  A  5.99283E-02

 BCC                          Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5360E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.31812E-01  A  6.81875E-02

 LIQUID                       Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.8707E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.05502E-01  A  1.94498E-01

 EXPERIMENT T=1203:DT  $1195.1:10  NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX  $0.194498:2E-2  NO=2
 EXPERIMENT W(BCC,A)=6.9E-2:DX  $6.81875E-2:2E-2  NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX  $5.99283E-2:2E-2  NO=4
ED_EXP: @@ Now equilibrium 4 is on the high B side
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: ba
   ... the command in full is BACK
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20:31




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1   TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.01820918E+04    2.01820918E+04    2.01820918E+04    0.00000000E+00
 V2     -2.90936108E+01   -2.90936108E+01   -2.90936108E+01    0.00000000E+00
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     2.36701045E+04    2.36701045E+04    2.36701045E+04    0.00000000E+00
 V16    -7.56540324E+00   -7.56540324E+00   -7.56540324E+00    0.00000000E+00
 V17     3.00342248E+03    3.00342248E+03    3.00342248E+03    0.00000000E+00
 V19     2.20133196E+04    2.20133196E+04    2.20133196E+04    0.00000000E+00
 V20    -6.72497818E+00   -6.72497818E+00   -6.72497818E+00    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :    7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO    8.21413189E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   3.73369632E-02



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.      10.0       0.6681      6.6807E-02
1 W(LIQUID,B)=0.408              0.4071      2.00E-02 -8.9916E-04 -4.4958E-02
1 W(BCC,B)=0.13                  0.1280      2.00E-02 -1.9512E-03 -9.7560E-02
2 T=1341                          1340.      10.0      -0.6301     -6.3010E-02
2 HTR=3727                        3759.      5.00E+02   31.69       6.3385E-02
3 T=1049                          1051.      10.0       2.137       0.2137
3 W(LIQUID,A)=0.27               0.2695      2.00E-02 -5.4230E-04 -2.7115E-02
3 W(BCC,A)=9.3E-2                9.0569E-02  2.00E-02 -2.4311E-03 -0.1216
4 T=1203                          1195.      10.0      -7.904      -0.7904
4 W(LIQUID,A)=0.19               0.1945      2.00E-02  4.4979E-03  0.2249
4 W(BCC,A)=6.9E-2                6.8188E-02  2.00E-02 -8.1248E-04 -4.0624E-02
4 W(FCC,A)=6E-2                  5.9928E-02  2.00E-02 -7.1681E-05 -3.5840E-03
5 T=726                           727.5      10.0       1.501       0.1501
5 X(BCC,B)=3.7E-2                3.8199E-02  2.00E-02  1.1988E-03  5.9941E-02
5 X(BCC#2,A)=0.114               0.1128      2.00E-02 -1.1687E-03 -5.8436E-02
6 X(BCC,B)=3.7E-2                3.7779E-02  2.00E-02  7.7870E-04  3.8935E-02
6 X(BCC#2,A)=0.114               0.1118      2.00E-02 -2.1691E-03 -0.1085
10 W(LIQUID,A)=2E-2              1.9541E-02  2.00E-02 -4.5856E-04 -2.2928E-02
11 W(LIQUID,A)=4.2E-2            4.1844E-02  2.00E-02 -1.5590E-04 -7.7951E-03
12 W(LIQUID,A)=6.5E-2            6.4983E-02  2.00E-02 -1.6862E-05 -8.4310E-04
13 W(LIQUID,A)=9.3E-2            9.2906E-02  2.00E-02 -9.3697E-05 -4.6848E-03
20 W(LIQUID,A)=0.104             0.1041      2.00E-02  6.5965E-05  3.2982E-03
20 W(FCC,A)=3.8E-2               3.7928E-02  2.00E-02 -7.1810E-05 -3.5905E-03
21 W(LIQUID,A)=0.136             0.1370      2.00E-02  9.7746E-04  4.8873E-02
21 W(FCC,A)=4.7E-2               4.6724E-02  2.00E-02 -2.7609E-04 -1.3805E-02
22 W(LIQUID,A)=0.187             0.1875      2.00E-02  5.0747E-04  2.5374E-02
22 W(FCC,A)=5.9E-2               5.8445E-02  2.00E-02 -5.5491E-04 -2.7745E-02
23 W(LIQUID,A)=0.245             0.2448      2.00E-02 -1.5069E-04 -7.5343E-03
23 W(BCC,A)=8.5E-2               8.2833E-02  2.00E-02 -2.1672E-03 -0.1084
```

```
PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    8.21413189E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    8.22231515E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    8.24025606E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    8.41459883E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    8.13854563E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    8.12128638E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    7.96555860E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    8.02217370E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    2.23904464E-01
  1  1.0000E+00   2  1.0000E+00   3  9.9684E-01   4  1.0013E+00   5  1.0004E+00
  6  1.0026E+00   7  9.9908E-01

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    2.14217788E-01
  1  1.0000E+00   2  9.9989E-01   3  9.9763E-01   4  1.0026E+00   5  1.0012E+00
  6  1.0043E+00   7  1.0027E+00

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    2.02688406E-01
  1  1.0001E+00   2  1.0000E+00   3  9.9857E-01   4  1.0047E+00   5  1.0024E+00
  6  1.0073E+00   7  1.0104E+00

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.86054744E-01
  1  1.0003E+00   2  1.0001E+00   3  1.0009E+00   4  1.0098E+00   5  1.0054E+00
  6  1.0128E+00   7  1.0246E+00

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.70130539E-01
  1  1.0007E+00   2  1.0004E+00   3  1.0050E+00   4  1.0192E+00   5  1.0109E+00
  6  1.0237E+00   7  1.0537E+00

      AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    1.67854613E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0074E+00   4  1.0249E+00   5  1.0142E+00
  6  1.0289E+00   7  1.0677E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   13 iterations
  1  1.0010E+00   2  1.0005E+00   3  1.0074E+00   4  1.0249E+00   5  1.0142E+00
  6  1.0289E+00   7  1.0677E+00

  1  6.3161E-02   2 -3.7856E-02   3 -8.1409E-02   4 -6.8335E-02   5  4.9923E-02
  6  2.5923E-01   7 -1.3946E-02   8 -9.1405E-02   9 -1.3190E-02  10  4.3922E-02
 11 -6.3822E-02  12 -8.0234E-02  13  1.6660E-01  14  3.1149E-02  15 -6.4319E-02
 16  8.0802E-03  17 -1.1993E-01  18 -1.7511E-02  19  4.0026E-04  20  7.0615E-03
 21 -6.1522E-04  22  4.9462E-03  23 -1.7573E-03  24  4.0977E-02  25 -2.3417E-02
 26 -2.5370E-03  27 -6.9024E-02  28  2.0311E-02  29 -7.1934E-02

               THE SUM OF SQUARES IS   1.67854613E-01
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20:31




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  14


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02022854E+04    2.01820918E+04    2.01820918E+04    2.48851232E-02
 V2     -2.91083428E+01   -2.90936108E+01   -2.90936108E+01    1.36093012E-02
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     2.38442417E+04    2.36701045E+04    2.36701045E+04    8.28181589E-02
 V16    -7.75412305E+00   -7.56540324E+00   -7.56540324E+00    2.55327975E-01
```

```
 V17     3.04598820E+03    3.00342248E+03    3.00342248E+03    2.36433798E-01
 V19     2.26500827E+04    2.20133196E+04    2.20133196E+04    4.73555705E-01
 V20    -7.18046737E+00   -6.72497818E+00   -6.72497818E+00    1.24878491E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.21413188E-01 TO   1.67854613E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   7.62975513E-03



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.      10.0      0.6316      6.3161E-02
1 W(LIQUID,B)=0.408              0.4072      2.00E-02 -7.5711E-04 -3.7856E-02
1 W(BCC,B)=0.13                  0.1284      2.00E-02 -1.6282E-03 -8.1409E-02
2 T=1341                          1340.      10.0     -0.6833     -6.8335E-02
2 HTR=3727                        3752.      5.00E+02   24.96      4.9923E-02
3 T=1049                          1052.      10.0       2.592      0.2592
3 W(LIQUID,A)=0.27               0.2697      2.00E-02 -2.7892E-04 -1.3946E-02
3 W(BCC,A)=9.3E-2                9.1172E-02  2.00E-02 -1.8281E-03 -9.1405E-02
4 T=1203                          1203.      10.0     -0.1319     -1.3190E-02
4 W(LIQUID,A)=0.19               0.1909      2.00E-02  8.7843E-04  4.3922E-02
4 W(BCC,A)=6.9E-2                6.7724E-02  2.00E-02 -1.2764E-03 -6.3822E-02
4 W(FCC,A)=6E-2                  5.8395E-02  2.00E-02 -1.6047E-03 -8.0234E-02
5 T=726                           727.7      10.0       1.666      0.1666
5 X(BCC,B)=3.7E-2                3.7623E-02  2.00E-02  6.2299E-04  3.1149E-02
5 X(BCC#2,A)=0.114               0.1127      2.00E-02 -1.2864E-03 -6.4319E-02
6 X(BCC,B)=3.7E-2                3.7162E-02  2.00E-02  1.6160E-04  8.0802E-03
6 X(BCC#2,A)=0.114               0.1116      2.00E-02 -2.3986E-03 -0.1199
10 W(LIQUID,A)=2E-2              1.9650E-02  2.00E-02 -3.5022E-04 -1.7511E-02
11 W(LIQUID,A)=4.2E-2            4.2008E-02  2.00E-02  8.0052E-06  4.0026E-04
12 W(LIQUID,A)=6.5E-2            6.5141E-02  2.00E-02  1.4123E-04  7.0615E-03
13 W(LIQUID,A)=9.3E-2            9.2988E-02  2.00E-02 -1.2304E-05 -6.1522E-04
20 W(LIQUID,A)=0.104             0.1041      2.00E-02  9.8925E-05  4.9462E-03
20 W(FCC,A)=3.8E-2               3.7965E-02  2.00E-02 -3.5145E-05 -1.7573E-03
21 W(LIQUID,A)=0.136             0.1368      2.00E-02  8.1954E-04  4.0977E-02
21 W(FCC,A)=4.7E-2               4.6532E-02  2.00E-02 -4.6834E-04 -2.3417E-02
22 W(LIQUID,A)=0.187             0.1869      2.00E-02 -5.0739E-05 -2.5370E-03
22 W(FCC,A)=5.9E-2               5.7620E-02  2.00E-02 -1.3805E-03 -6.9024E-02
23 W(LIQUID,A)=0.245             0.2454      2.00E-02  4.0622E-04  2.0311E-02
23 W(BCC,A)=8.5E-2               8.3561E-02  2.00E-02 -1.4387E-03 -7.1934E-02


PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Now optimize all parameters and all experiments
PARROT: l-a-v
   ... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02022854E+04    2.01820918E+04    2.01820918E+04    2.48851232E-02
 V2     -2.91083428E+01   -2.90936108E+01   -2.90936108E+01    1.36093012E-02
 V11    -2.18127452E+04
 V12     1.55559572E+01
 V15     2.38442417E+04    2.36701045E+04    2.36701045E+04    8.28181589E-02
 V16    -7.75412305E+00   -7.56540324E+00   -7.56540324E+00    2.55327975E-01
 V17     3.04598820E+03    3.00342248E+03    3.00342248E+03    2.36433798E-01
 V19     2.26500827E+04    2.20133196E+04    2.20133196E+04    4.73555705E-01
 V20    -7.18046737E+00   -6.72497818E+00   -6.72497818E+00    1.24878491E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.21413188E-01 TO   1.67854613E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   7.62975513E-03
PARROT: s-o-v 11-12
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1193.6      LIQUID A2B BCC
   2 AINV   2   1.    1340.3      LIQUID A2B
   3 AINV   2   1.    1051.6      LIQUID A2B BCC
   4 AINV   2   1.    1202.9      LIQUID BCC FCC
   5 AINV   2   1.     727.7      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    2   1.    1594.0      LIQUID FCC
  11 ALF    2   1.    1548.0      LIQUID FCC
  12 ALF    2   1.    1499.0      LIQUID FCC
  13 ALF    2   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA   < unused >  1573.0      LIQUID
 101 AA   < unused >  1573.0      LIQUID
 102 AA   < unused >  1573.0      LIQUID
 103 AA   < unused >  1573.0      LIQUID
 104 AA   < unused >  1573.0      LIQUID
 105 AA   < unused >  1573.0      LIQUID
 106 AA   < unused >  1573.0      LIQUID
 107 AA   < unused >  1573.0      LIQUID
 108 AA   < unused >  1573.0      LIQUID
 110 AH   < unused >  1773.0      LIQUID
 111 AH   < unused >  1773.0      LIQUID
 112 AH   < unused >  1773.0      LIQUID
 113 AH   < unused >  1773.0      LIQUID
 114 AH   < unused >  1773.0      LIQUID
 115 AH   < unused >  1773.0      LIQUID
 116 AH   < unused >  1773.0      LIQUID
 117 AH   < unused >  1773.0      LIQUID
```

```
 118 AH    < unused >  1773.0      LIQUID
ED_EXP: s-we 1 100-118
   ... the command in full is SET_WEIGHT
ED_EXP: s-e 1
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                      1 , label AINV
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1193.6      LIQUID A2B BCC
   2 AINV   2   1.    1340.3      LIQUID A2B
   3 AINV   2   1.    1051.6      LIQUID A2B BCC
   4 AINV   2   1.    1202.9      LIQUID BCC FCC
   5 AINV   2   1.     727.7      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    2   1.    1594.0      LIQUID FCC
  11 ALF    2   1.    1548.0      LIQUID FCC
  12 ALF    2   1.    1499.0      LIQUID FCC
  13 ALF    2   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     2   1.    1773.0      LIQUID
 116 AH     2   1.    1773.0      LIQUID
 117 AH     2   1.    1773.0      LIQUID
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    5.15879918E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0000E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    5.16684214E-01
  1  1.0011E+00   2  1.0005E+00   3  1.0000E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    5.18528647E-01
  1  1.0010E+00   2  1.0006E+00   3  1.0000E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    5.10059302E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    5.14690131E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0001E+00   5  1.0074E+00
  6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10340685E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0075E+00
  6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10048087E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0250E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10055130E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0250E+00   7  1.0143E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10212338E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0250E+00   7  1.0142E+00   8  1.0290E+00   9  1.0677E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10033022E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0250E+00   7  1.0142E+00   8  1.0289E+00   9  1.0678E+00

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    4.31534544E-01
  1  1.0007E+00   2  1.0011E+00   3  1.0017E+00   4  9.9872E-01   5  1.0073E+00
  6  1.0251E+00   7  1.0142E+00   8  1.0289E+00   9  1.0678E+00

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    3.88006645E-01
  1  1.0007E+00   2  1.0016E+00   3  1.0015E+00   4  9.9831E-01   5  1.0076E+00
  6  1.0269E+00   7  1.0145E+00   8  1.0283E+00   9  1.0674E+00

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    3.46571329E-01
  1  1.0012E+00   2  1.0021E+00   3  1.0017E+00   4  9.9707E-01   5  1.0078E+00
  6  1.0307E+00   7  1.0152E+00   8  1.0271E+00   9  1.0665E+00

      AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    2.88315117E-01
  1  1.0019E+00   2  1.0031E+00   3  1.0011E+00   4  9.9524E-01   5  1.0092E+00
  6  1.0382E+00   7  1.0164E+00   8  1.0246E+00   9  1.0647E+00

      AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    2.01092406E-01
  1  1.0035E+00   2  1.0050E+00   3  1.0003E+00   4  9.9135E-01   5  1.0119E+00
  6  1.0533E+00   7  1.0190E+00   8  1.0194E+00   9  1.0612E+00

      AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    9.39326709E-02
  1  1.0066E+00   2  1.0086E+00   3  9.9812E-01   4  9.8393E-01   5  1.0177E+00
  6  1.0836E+00   7  1.0240E+00   8  1.0095E+00   9  1.0548E+00
```

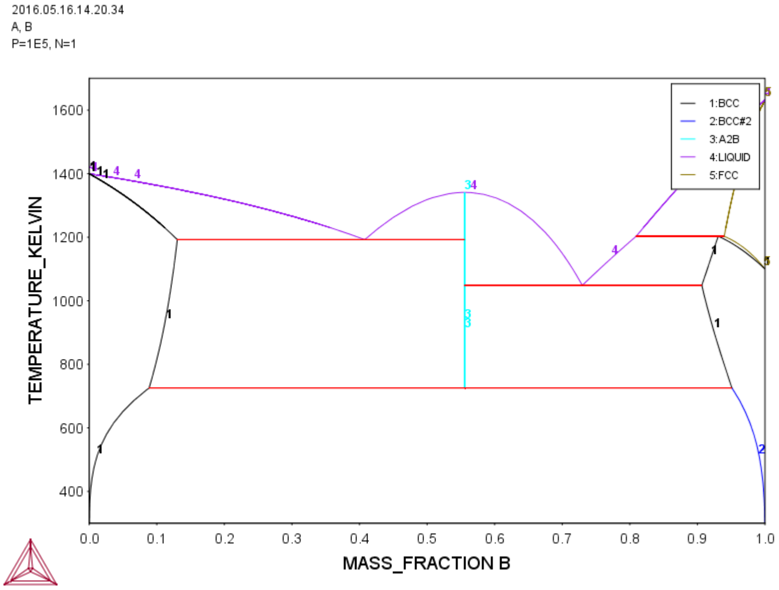
```
      AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    6.73924422E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   16 iterations
  1  1.0093E+00   2  1.0115E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

  1 -5.7709E-02   2 -9.3404E-03   3  1.4435E-02   4  2.0965E-02   5 -2.5772E-02
  6 -5.2196E-02   7  1.9264E-02   8  2.6907E-02   9  1.1430E-02  10  2.7509E-02
 11  8.8336E-03  12  1.3392E-02  13 -4.8280E-02  14  2.2178E-02  15  5.2234E-03
 16  2.9005E-02  17  2.1915E-02  18 -2.1795E-02  19 -7.8107E-03  20 -4.4451E-03
 21 -1.5094E-02  22 -1.0366E-02  23  1.5822E-02  24  2.4683E-02  25  1.5219E-02
 26 -1.4822E-02  27  2.0407E-02  28 -1.2809E-02  29  1.5407E-02  30 -9.5946E-03
 31 -1.6846E-02  32  2.7408E-02  33  8.6976E-02  34  1.2428E-01  35  1.0162E-01
 36 -1.7386E-02  37  7.0520E-02  38 -1.9513E-02  39  1.6094E-02  40  4.5500E-02
 41  4.8219E-02  42  4.6251E-02  43  4.1594E-02  44  3.4251E-02  45  2.2219E-02
 46  7.5004E-03  47 -1.1906E-02

               THE SUM OF SQUARES IS    6.73924422E-02
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:20:31




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  17


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820918E+04    2.01820918E+04    3.02498426E-02
 V2     -2.94290453E+01   -2.90936108E+01   -2.90936108E+01    2.30117855E-02
 V11    -2.17328114E+04   -2.18127452E+04   -2.18127452E+04    3.47139484E-02
 V12     1.52102756E+01    1.55559572E+01    1.55559572E+01    5.38555420E-02
 V15     2.42012673E+04    2.36701045E+04    2.36701045E+04    8.60926362E-02
 V16    -8.38545778E+00   -7.56540324E+00   -7.56540324E+00    2.83695736E-01
 V17     3.08774252E+03    3.00342248E+03    3.00342248E+03    2.37803227E-01
 V19     2.20600539E+04    2.20133196E+04    2.20133196E+04    4.87694893E-01
 V20    -7.07096129E+00   -6.72497818E+00   -6.72497818E+00    1.27666199E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15879918E-01 TO   6.73924422E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.77348532E-03



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.      10.0      -0.5771     -5.7709E-02
1 W(LIQUID,B)=0.408              0.4078     2.00E-02 -1.8681E-04 -9.3404E-03
1 W(BCC,B)=0.13                  0.1303     2.00E-02  2.8870E-04  1.4435E-02
2 T=1341                          1341.      10.0       0.2096      2.0965E-02
2 HTR=3727                        3714.      5.00E+02  -12.89      -2.5772E-02
3 T=1049                          1048.      10.0      -0.5220     -5.2196E-02
3 W(LIQUID,A)=0.27               0.2704     2.00E-02  3.8528E-04  1.9264E-02
3 W(BCC,A)=9.3E-2                9.3538E-02  2.00E-02  5.3815E-04  2.6907E-02
4 T=1203                          1203.      10.0       0.1143      1.1430E-02
4 W(LIQUID,A)=0.19               0.1906     2.00E-02  5.5018E-04  2.7509E-02
4 W(BCC,A)=6.9E-2                6.9177E-02  2.00E-02  1.7667E-04  8.8336E-03
4 W(FCC,A)=6E-2                  6.0268E-02  2.00E-02  2.6783E-04  1.3392E-02
5 T=726                           725.5      10.0      -0.4828     -4.8280E-02
5 X(BCC,B)=3.7E-2                3.7444E-02  2.00E-02  4.4356E-04  2.2178E-02
5 X(BCC#2,A)=0.114               0.1141     2.00E-02  1.0447E-04  5.2234E-03
6 X(BCC,B)=3.7E-2                3.7580E-02  2.00E-02  5.8011E-04  2.9005E-02
6 X(BCC#2,A)=0.114               0.1144     2.00E-02  4.3830E-04  2.1915E-02
10 W(LIQUID,A)=2E-2              1.9564E-02  2.00E-02 -4.3589E-04 -2.1795E-02
11 W(LIQUID,A)=4.2E-2            4.1844E-02  2.00E-02 -1.5621E-04 -7.8107E-03
12 W(LIQUID,A)=6.5E-2            6.4911E-02  2.00E-02 -8.8902E-05 -4.4451E-03
13 W(LIQUID,A)=9.3E-2            9.2698E-02  2.00E-02 -3.0187E-04 -1.5094E-02
20 W(LIQUID,A)=0.104             0.1038     2.00E-02 -2.0731E-04 -1.0366E-02
20 W(FCC,A)=3.8E-2               3.8316E-02  2.00E-02  3.1645E-04  1.5822E-02
21 W(LIQUID,A)=0.136             0.1365     2.00E-02  4.9366E-04  2.4683E-02
21 W(FCC,A)=4.7E-2               4.7304E-02  2.00E-02  3.0438E-04  1.5219E-02
22 W(LIQUID,A)=0.187             0.1867     2.00E-02 -2.9644E-04 -1.4822E-02
22 W(FCC,A)=5.9E-2               5.9408E-02  2.00E-02  4.0813E-04  2.0407E-02
23 W(LIQUID,A)=0.245             0.2447     2.00E-02 -2.5617E-04 -1.2809E-02
23 W(BCC,A)=8.5E-2               8.5308E-02  2.00E-02  3.0814E-04  1.5407E-02
100 ACR(B)=0.94                  0.9397     2.85E-02 -2.7309E-04 -9.5946E-03
101 ACR(B)=0.84                  0.8395     2.82E-02 -4.7482E-04 -1.6846E-02
102 ACR(B)=0.74                  0.7408     2.81E-02  7.6893E-04  2.7408E-02
103 ACR(B)=0.64                  0.6424     2.81E-02  2.4411E-03  8.6976E-02
104 ACR(B)=0.54                  0.5435     2.82E-02  3.5079E-03  0.1243
105 ACR(B)=0.44                  0.4429     2.85E-02  2.9003E-03  0.1016
106 ACR(B)=0.34                  0.3395     2.90E-02 -5.0467E-04 -1.7386E-02
107 ACR(B)=0.23                  0.2321     2.97E-02  2.0948E-03  7.0520E-02
108 ACR(B)=0.12                  0.1194     3.06E-02 -5.9712E-04 -1.9513E-02
110 HMR(LIQUID)=-1964            -1956.      5.00E+02   8.047       1.6094E-02
111 HMR(LIQUID)=-3500            -3477.      5.00E+02   22.75       4.5500E-02
112 HMR(LIQUID)=-4588            -4564.      5.00E+02   24.11       4.8219E-02
```

```
113 HMR(LIQUID)=-5239            -5216.      5.00E+02   23.13      4.6251E-02
114 HMR(LIQUID)=-5454            -5433.      5.00E+02   20.80      4.1594E-02
115 HMR(LIQUID)=-5233            -5216.      5.00E+02   17.13      3.4251E-02
116 HMR(LIQUID)=-4575            -4564.      5.00E+02   11.11      2.2219E-02
117 HMR(LIQUID)=-3481            -3477.      5.00E+02   3.750      7.5004E-03
118 HMR(LIQUID)=-1950            -1956.      5.00E+02  -5.953     -1.1906E-02


PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram a final time.
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC
  ** BCC#2
 Calculated..                      2  equilibria
 Terminating at axis limit.
```

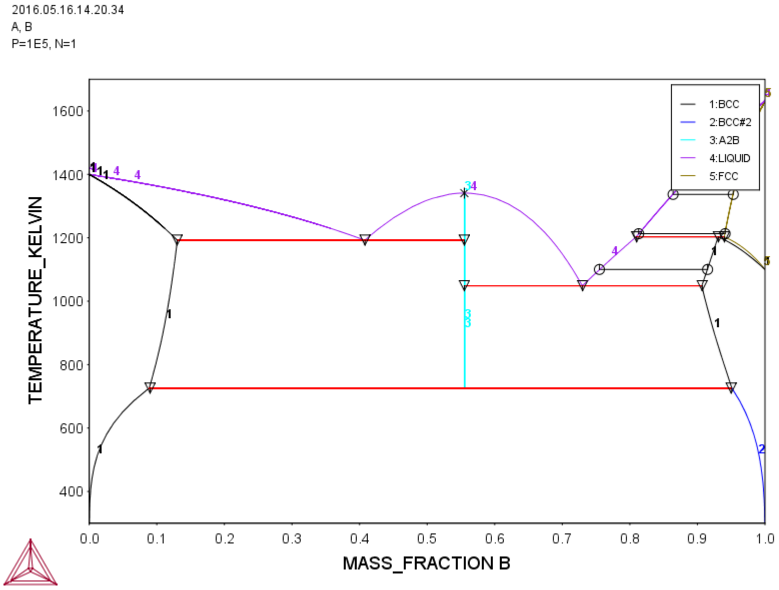
```
Phase region boundary   2 at:   7.141E-01  3.000E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria

Phase region boundary   3 at:   6.819E-01  7.255E+02
 ** A2B
    BCC
 ** BCC#2

Phase region boundary   4 at:   3.626E-01  7.255E+02
 ** A2B
    BCC
Calculated.                     15  equilibria

Phase region boundary   5 at:   3.771E-01  1.192E+03
 ** LIQUID
 ** A2B
    BCC

Phase region boundary   6 at:   2.828E-01  1.192E+03
 ** LIQUID
    BCC
Calculated                     28  equilibria

Phase region boundary   7 at:   4.863E-01  1.192E+03
 ** LIQUID
    A2B
Calculated.                     28  equilibria

Phase region boundary   8 at:   6.500E-01  1.048E+03
 ** LIQUID
    A2B
 ** BCC

Phase region boundary   9 at:   7.639E-01  1.048E+03
    A2B
 ** BCC
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.273E-01  1.048E+03
    LIQUID
 ** BCC
Calculated.                      8  equilibria

Phase region boundary  11 at:   8.748E-01  1.203E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.799E-01  1.203E+03
    LIQUID
 ** FCC
Calculated                     35  equilibria

Phase region boundary  13 at:   9.353E-01  1.203E+03
    BCC
 ** FCC
Calculated                     24  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
```

```
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.647E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  26 at:   3.647E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.647E-01  7.700E+02
 ** A2B
    BCC
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.910E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  29 at:   7.910E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.910E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.448E-01  1.230E+03
 ** LIQUID
    BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.448E-01  1.230E+03
 ** LIQUID
    BCC
Calculated                     26  equilibria

Phase region boundary  33 at:   8.858E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.858E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                     29  equilibria

Phase region boundary  35 at:   6.415E-03  1.397E+03
    LIQUID
 ** BCC
Calculated                     13  equilibria

Phase region boundary  36 at:   6.415E-03  1.397E+03
    LIQUID
 ** BCC
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.299E-01  1.244E+03
    LIQUID
 ** BCC
Calculated                     23  equilibria

Phase region boundary  38 at:   2.299E-01  1.244E+03
    LIQUID
 ** BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.240E+03
    LIQUID
 ** A2B
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.122E-01  1.240E+03
    LIQUID
 ** A2B
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   9.927E-01  1.613E+03
    LIQUID
 ** FCC
Calculated.                     20  equilibria
Terminating at known equilibrium

Phase region boundary  42 at:   9.927E-01  1.613E+03
    LIQUID
 ** FCC
Calculated                      9  equilibria
```

```
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                        1  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

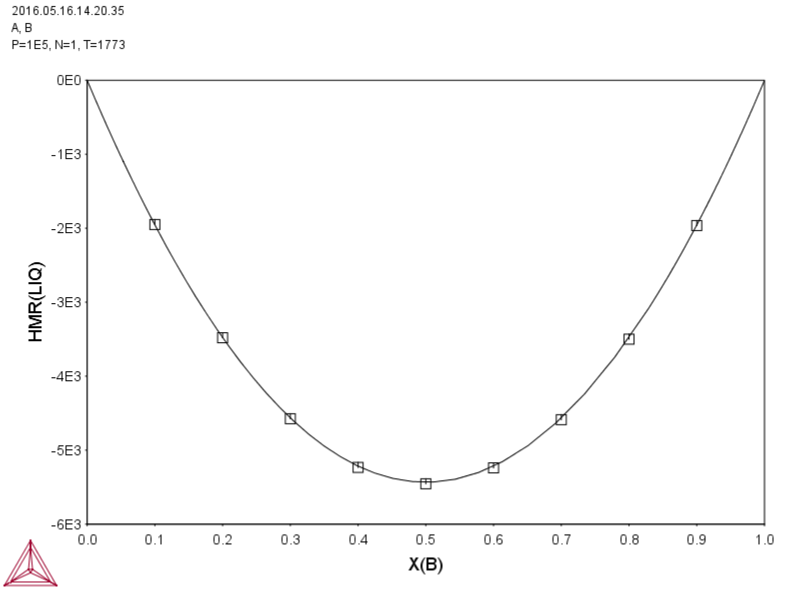


```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ Add the experimental data
POST: a-e-d y exp36 0; 1
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

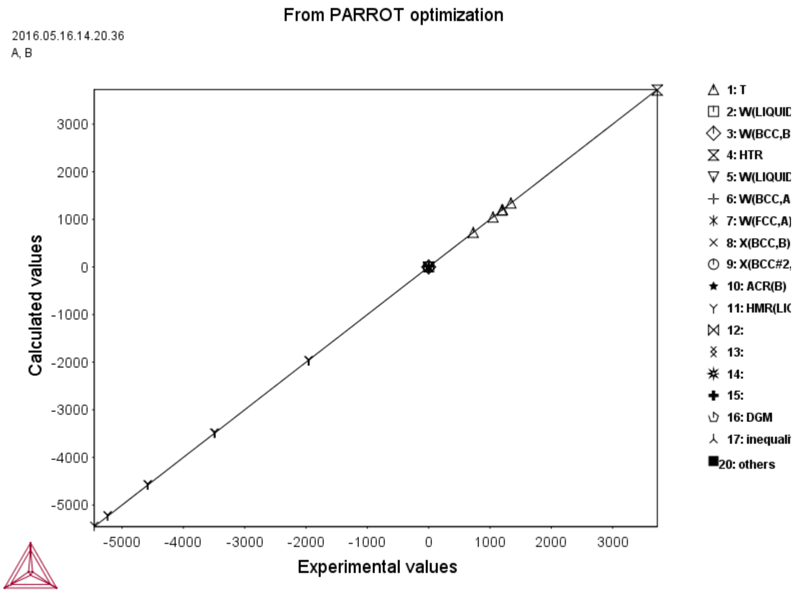


```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
   ... the command in full is BACK
POLY_3: read,,,
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-c t=1773
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
POLY_3: sh hmr
   ... the command in full is SHOW_VALUE
 HMR=13116.476
POLY_3: l-st c
```

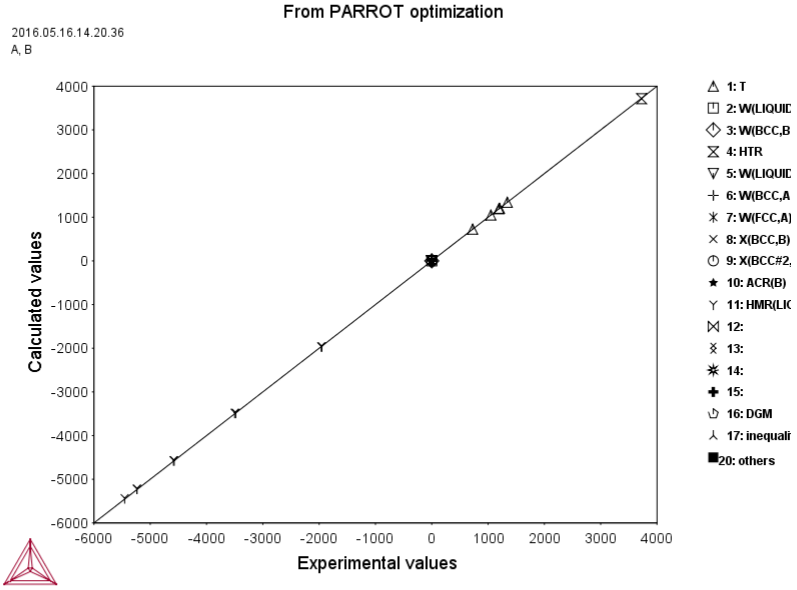
```
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 A                        ENTERED   SER
 B                        ENTERED   SER
POLY_3: s-r-s a liq * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s b liq * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: save tcex36h y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.123400
...OK

 Phase Region from   0.123400     for:
     LIQUID
 Global test at  3.23400E-01 .... OK
 Global test at  5.73400E-01 .... OK
 Global test at  8.23400E-01 .... OK
 Global test at  9.53400E-01 .... OK
 Global test at  1.00000E+00 .... OK
 Terminating at    1.00000
 Calculated    51 equilibria

 Phase Region from   0.123400     for:
     LIQUID
 Global test at  8.34000E-02 .... OK
 Global test at  3.34000E-02 .... OK
 Terminating at   0.250000E-11
 Calculated    28 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36h.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x x(b)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y hmr(liq)
   ... the command in full is SET_DIAGRAM_AXIS
POST: a-e-d y exp36 0; 2
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-result gra pexp36 1,
   ... the command in full is LIST_RESULT
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is PLOT_DIAGRAM
```



```
POST: s-s-s y n -6000 4000
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s x n -6000 4000
   ... the command in full is SET_SCALING_STATUS
POST: pl
   ... the command in full is PLOT_DIAGRAM
```



```
POST: b
   ... the command in full is BACK
PARROT: set-inter
   ... the command in full is SET_INTERACTIVE
PARROT: set-inter
   ... the command in full is SET_INTERACTIVE
PARROT:
```

tcex36a-tcex36b

```
PARROT:AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tcex36b.TCM"PARROT: s-s-f tcex36
   ... the command in full is SET_STORE_FILE
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
   ... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820918E+04    2.01820918E+04    3.02498426E-02
 V2     -2.94290453E+01   -2.90936108E+01   -2.90936108E+01    2.30117855E-02
 V11    -2.17328114E+04   -2.18127452E+04   -2.18127452E+04    3.47139484E-02
 V12     1.52102756E+01    1.55559572E+01    1.55559572E+01    5.38555420E-02
 V15     2.42012673E+04    2.36701045E+04    2.36701045E+04    8.60926362E-02
 V16    -8.38545778E+00   -7.56540324E+00   -7.56540324E+00    2.83695736E-01
 V17     3.08774252E+03    3.00342248E+03    3.00342248E+03    2.37803227E-01
 V19     2.20600539E+04    2.20133196E+04    2.20133196E+04    4.87694893E-01
 V20    -7.07096129E+00   -6.72497818E+00   -6.72497818E+00    1.27666199E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15879918E-01 TO   6.73924422E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.77348532E-03
PARROT: @@ Set alt mode to start
PARROT: s-alt Y
   ... the command in full is SET_ALTERNATE_MODE
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV *alt*  1.0  1193.0      LIQUID A2B BCC
   2 AINV *alt*  1.0  1341.0      LIQUID A2B
   3 AINV *alt*  1.0  1049.0      LIQUID A2B BCC
   4 AINV *alt*  1.0  1203.0      LIQUID BCC FCC
   5 AINV *alt*  1.0   726.0      A2B BCC BCC#2
   6 AINV *alt*  1.0   726.0      BCC BCC#2
 Failed using alternate for FCC#1                      setting weight to zero
  10 ALF  *alt*  1.0  1594.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  11 ALF  *alt*  1.0  1548.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  12 ALF  *alt*  1.0  1499.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  13 ALF  *alt*  1.0  1438.0      LIQUID FCC
  20 ATIE *alt*  1.0  1413.0      LIQUID FCC
  21 ATIE *alt*  1.0  1337.0      LIQUID FCC
  22 ATIE *alt*  1.0  1213.0      LIQUID FCC
  23 ATIE *alt*  1.0  1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     2   1.    1773.0      LIQUID
 116 AH     2   1.    1773.0      LIQUID
 117 AH     2   1.    1773.0      LIQUID
 118 AH     2   1.    1773.0      LIQUID
 Number of alternate equilibria                     14
ED_EXP: @@ Equilibra with label ALF cannot use alt mode
ED_EXP: s-we 0 alf
   ... the command in full is SET_WEIGHT
 Changed weight on                        4  equilibria.
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes of weights before leaving editor
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ Optimize zero times as a check
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:29




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
```

```
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =    0    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820918E+04    2.01820918E+04    3.02498426E-02
 V2     -2.94290453E+01   -2.90936108E+01   -2.90936108E+01    2.30117855E-02
 V11    -2.17328114E+04   -2.18127452E+04   -2.18127452E+04    3.47139484E-02
 V12     1.52102756E+01    1.55559572E+01    1.55559572E+01    5.38555420E-02
 V15     2.42012673E+04    2.36701045E+04    2.36701045E+04    8.60926362E-02
 V16    -8.38545778E+00   -7.56540324E+00   -7.56540324E+00    2.83695736E-01
 V17     3.08774252E+03    3.00342248E+03    3.00342248E+03    2.37803227E-01
 V19     2.20600539E+04    2.20133196E+04    2.20133196E+04    4.87694893E-01
 V20    -7.07096129E+00   -6.72497818E+00   -6.72497818E+00    1.27666199E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15879918E-01 TO   8.89279099E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   2.34020816E-03

 Number of alternate equilibria                     10


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                       0.00
   2 Alternate equilibrium calc                                       0.19
2 HTR=3727                        3714.      5.00E+02  -12.89     -2.5772E-02
   3 Alternate equilibrium calc                                       0.00
   4 Alternate equilibrium calc                                       0.00
   5 Alternate equilibrium calc                                       0.01
   6 Alternate equilibrium calc                                       0.01
  20 Alternate equilibrium calc                                       0.01
  21 Alternate equilibrium calc                                       0.00
  22 Alternate equilibrium calc                                       0.01
  23 Alternate equilibrium calc                                       0.00
100 ACR(B)=0.94                  0.9397      2.85E-02 -2.7309E-04 -9.5946E-03
101 ACR(B)=0.84                  0.8395      2.82E-02 -4.7482E-04 -1.6846E-02
102 ACR(B)=0.74                  0.7408      2.81E-02  7.6893E-04  2.7408E-02
103 ACR(B)=0.64                  0.6424      2.81E-02  2.4411E-03  8.6976E-02
104 ACR(B)=0.54                  0.5435      2.82E-02  3.5079E-03  0.1243
105 ACR(B)=0.44                  0.4429      2.85E-02  2.9003E-03  0.1016
106 ACR(B)=0.34                  0.3395      2.90E-02 -5.0467E-04 -1.7386E-02
107 ACR(B)=0.23                  0.2321      2.97E-02  2.0948E-03  7.0520E-02
108 ACR(B)=0.12                  0.1194      3.06E-02 -5.9712E-04 -1.9513E-02
110 HMR(LIQUID)=-1964            -1956.      5.00E+02   8.047      1.6094E-02
111 HMR(LIQUID)=-3500            -3477.      5.00E+02   22.75      4.5500E-02
112 HMR(LIQUID)=-4588            -4564.      5.00E+02   24.11      4.8219E-02
113 HMR(LIQUID)=-5239            -5216.      5.00E+02   23.13      4.6251E-02
114 HMR(LIQUID)=-5454            -5433.      5.00E+02   20.80      4.1594E-02
115 HMR(LIQUID)=-5233            -5216.      5.00E+02   17.13      3.4251E-02
116 HMR(LIQUID)=-4575            -4564.      5.00E+02   11.11      2.2219E-02
117 HMR(LIQUID)=-3481            -3477.      5.00E+02   3.750      7.5004E-03
118 HMR(LIQUID)=-1950            -1956.      5.00E+02  -5.953     -1.1906E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Note only one error from alternate calculations. This error represents
PARROT: @@ the difference in chemical potentials of the phases.
PARROT: @@ Experiments with just one phase is calculated as normal.
PARROT: @@ Next command supresses listing of parameters.
PARROT: s-o-l 1 Y Y N n N
   ... the command in full is SET_OUTPUT_LEVELS
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


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           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:29




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =    0    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820918E+04    2.01820918E+04    3.02498426E-02
 V2     -2.94290453E+01   -2.90936108E+01   -2.90936108E+01    2.30117855E-02
 V11    -2.17328114E+04   -2.18127452E+04   -2.18127452E+04    3.47139484E-02
 V12     1.52102756E+01    1.55559572E+01    1.55559572E+01    5.38555420E-02
 V15     2.42012673E+04    2.36701045E+04    2.36701045E+04    8.60926362E-02
 V16    -8.38545778E+00   -7.56540324E+00   -7.56540324E+00    2.83695736E-01
 V17     3.08774252E+03    3.00342248E+03    3.00342248E+03    2.37803227E-01
```

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 V19     2.20600539E+04    2.20133196E+04    2.20133196E+04    4.87694893E-01
 V20    -7.07096129E+00   -6.72497818E+00   -6.72497818E+00    1.27666199E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15879918E-01 TO   8.89279099E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   2.34020816E-03

 Number of alternate equilibria                     10

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0369117E+04
   4 V2        48000000 -2.9429045E+01
  13 V11       48000000 -2.1732811E+04
  14 V12       48000000  1.5210276E+01
  17 V15       48000000  2.4201267E+04
  18 V16       48000000 -8.3854578E+00
  19 V17       48000000  3.0877425E+03
  21 V19       48000000  2.2060054E+04
  22 V20       48000000 -7.0709613E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                    0.00
   2 Alternate equilibrium calc                                    0.19
2 HTR=3727                    3714.      5.00E+02  -12.89     -2.5772E-02
   3 Alternate equilibrium calc                                    0.00
   4 Alternate equilibrium calc                                    0.00
   5 Alternate equilibrium calc                                    0.01
   6 Alternate equilibrium calc                                    0.01
  20 Alternate equilibrium calc                                    0.01
  21 Alternate equilibrium calc                                    0.00
  22 Alternate equilibrium calc                                    0.01
  23 Alternate equilibrium calc                                    0.00
100 ACR(B)=0.94              0.9397      2.85E-02 -2.7309E-04 -9.5946E-03
101 ACR(B)=0.84              0.8395      2.82E-02 -4.7482E-04 -1.6846E-02
102 ACR(B)=0.74              0.7408      2.81E-02  7.6893E-04  2.7408E-02
103 ACR(B)=0.64              0.6424      2.81E-02  2.4411E-03  8.6976E-02
104 ACR(B)=0.54              0.5435      2.82E-02  3.5079E-03  0.1243
105 ACR(B)=0.44              0.4429      2.85E-02  2.9003E-03  0.1016
106 ACR(B)=0.34              0.3395      2.90E-02 -5.0467E-04 -1.7386E-02
107 ACR(B)=0.23              0.2321      2.97E-02  2.0948E-03  7.0520E-02
108 ACR(B)=0.12              0.1194      3.06E-02 -5.9712E-04 -1.9513E-02
110 HMR(LIQUID)=-1964        -1956.      5.00E+02   8.047      1.6094E-02
111 HMR(LIQUID)=-3500        -3477.      5.00E+02   22.75      4.5500E-02
112 HMR(LIQUID)=-4588        -4564.      5.00E+02   24.11      4.8219E-02
113 HMR(LIQUID)=-5239        -5216.      5.00E+02   23.13      4.6251E-02
114 HMR(LIQUID)=-5454        -5433.      5.00E+02   20.80      4.1594E-02
115 HMR(LIQUID)=-5233        -5216.      5.00E+02   17.13      3.4251E-02
116 HMR(LIQUID)=-4575        -4564.      5.00E+02   11.11      2.2219E-02
117 HMR(LIQUID)=-3481        -3477.      5.00E+02   3.750      7.5004E-03
118 HMR(LIQUID)=-1950        -1956.      5.00E+02  -5.953     -1.1906E-02


PARROT:
PARROT: @@ Now optimize
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    8.89279099E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    8.89950288E-02
```

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  1  1.0094E+00   2  1.0115E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    8.89370493E-02
  1  1.0093E+00   2  1.0116E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    8.79489886E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    8.85893317E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7788E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79262642E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79317664E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
  6  1.1085E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79245152E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
  6  1.1084E+00   7  1.0282E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79198012E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
  6  1.1084E+00   7  1.0282E+00   8  1.0022E+00   9  1.0514E+00

     AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79216928E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
  6  1.1084E+00   7  1.0282E+00   8  1.0022E+00   9  1.0515E+00

     AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    6.30012576E-02
  1  1.0090E+00   2  1.0115E+00   3  1.0000E+00   4  9.7542E-01   5  1.0226E+00
  6  1.1084E+00   7  1.0282E+00   8  1.0022E+00   9  1.0514E+00

     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    6.00250613E-02
  1  1.0062E+00   2  1.0109E+00   3  9.9912E-01   4  9.7423E-01   5  1.0235E+00
  6  1.1105E+00   7  1.0290E+00   8  1.0016E+00   9  1.0501E+00

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    5.93161822E-02
  1  1.0057E+00   2  1.0092E+00   3  9.9970E-01   4  9.7424E-01   5  1.0255E+00
  6  1.1178E+00   7  1.0318E+00   8  1.0004E+00   9  1.0481E+00

     AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88760571E-02
  1  1.0049E+00   2  1.0059E+00   3  9.9988E-01   4  9.7463E-01   5  1.0295E+00
  6  1.1320E+00   7  1.0370E+00   8  9.9745E-01   9  1.0425E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   13 iterations
  1  1.0049E+00   2  1.0059E+00   3  9.9988E-01   4  9.7463E-01   5  1.0295E+00
  6  1.1320E+00   7  1.0370E+00   8  9.9745E-01   9  1.0425E+00

  1  6.9039E-03   2  6.9039E-03   3  1.5738E-03   4  2.6800E-03   5  1.3310E-01
  6 -1.3983E-01   7 -1.4164E-03   8  7.6472E-03   9  7.6472E-03  10 -1.0561E-04
 11  3.2960E-03  12  2.1369E-03  13  2.5829E-04  14  3.0760E-03  15  6.0633E-04
 16  1.2976E-03  17  1.2976E-03  18  2.3664E-05  19  1.6822E-03  20  2.3664E-05
 21  1.6822E-03  22 -2.0443E-03  23  1.7694E-03  24  3.4709E-03  25  3.3350E-04
 26 -2.5368E-03  27  3.2555E-03  28 -1.4427E-03  29  3.8328E-03  30 -1.3478E-02
 31 -3.0855E-02  32 -6.3336E-04  33  4.3684E-02  34  6.7408E-02  35  3.5765E-02
 36 -8.4872E-02  37  1.1726E-02  38 -5.6892E-02  39  2.1632E-03  40  2.0734E-02
 41  1.5714E-02  42  9.1017E-03  43  2.8977E-03  44 -2.8983E-03  45 -1.0286E-02
 46 -1.7266E-02  47 -2.5837E-02

              THE SUM OF SQUARES IS   5.88760571E-02
PARROT: cont 30
   ... the command in full is CONTINUE_OPTIMIZATION

 It is safe to CONTINUE only after TOO MANY ITERATIONS
 and no change in variables and experiments ...
 Now anything can happen ...

PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


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          OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:29




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  14


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE               START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02809885E+04    2.01820918E+04    2.01820918E+04    7.95747010E-02
 V2     -2.92651699E+01   -2.90936108E+01   -2.90936108E+01    3.44415373E-01
 V11    -2.18102047E+04   -2.18127452E+04   -2.18127452E+04    3.96943915E-02
 V12     1.51613087E+01    1.55559572E+01    1.55559572E+01    5.70071432E-02
 V15     2.43675665E+04    2.36701045E+04    2.36701045E+04    6.28240698E-01
 V16    -8.56377518E+00   -7.56540324E+00   -7.56540324E+00    2.32375383E+00
 V17     3.11464876E+03    3.00342248E+03    3.00342248E+03    1.51251851E+00
 V19     2.19570764E+04    2.20133196E+04    2.20133196E+04    4.62338048E+00
 V20    -7.01093190E+00   -6.72497818E+00   -6.72497818E+00    1.17285936E+01
```
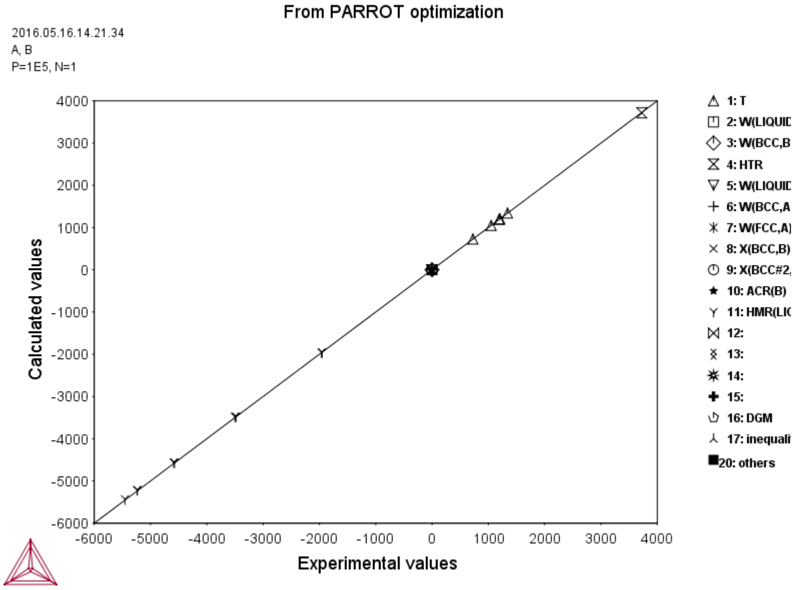

```
 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.89279099E-02 TO   5.88760571E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.54936992E-03

 Number of alternate equilibria                     10

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0280989E+04
   4 V2        48000000 -2.9265170E+01
  13 V11       48000000 -2.1810205E+04
  14 V12       48000000  1.5161309E+01
  17 V15       48000000  2.4367567E+04
  18 V16       48000000 -8.5637752E+00
  19 V17       48000000  3.1146488E+03
  21 V19       48000000  2.1957076E+04
  22 V20       48000000 -7.0109319E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                       0.01
   2 Alternate equilibrium calc                                       0.19
2 HTR=3727                        3726.      5.00E+02 -0.7082     -1.4164E-03
   3 Alternate equilibrium calc                                       0.01
   4 Alternate equilibrium calc                                       0.00
   5 Alternate equilibrium calc                                       0.00
   6 Alternate equilibrium calc                                       0.00
  20 Alternate equilibrium calc                                       0.00
  21 Alternate equilibrium calc                                       0.00
  22 Alternate equilibrium calc                                       0.00
  23 Alternate equilibrium calc                                       0.00
100 ACR(B)=0.94                  0.9396      2.85E-02 -3.8404E-04 -1.3478E-02
101 ACR(B)=0.84                  0.8391      2.82E-02 -8.7121E-04 -3.0855E-02
102 ACR(B)=0.74                  0.7400      2.81E-02 -1.7806E-05 -6.3336E-04
103 ACR(B)=0.64                  0.6412      2.81E-02  1.2286E-03  4.3684E-02
104 ACR(B)=0.54                  0.5419      2.83E-02  1.9060E-03  6.7408E-02
105 ACR(B)=0.44                  0.4410      2.86E-02  1.0218E-03  3.5765E-02
106 ACR(B)=0.34                  0.3375      2.90E-02 -2.4631E-03 -8.4872E-02
107 ACR(B)=0.23                  0.2303      2.96E-02  3.4765E-04  1.1726E-02
108 ACR(B)=0.12                  0.1183      3.05E-02 -1.7336E-03 -5.6892E-02
110 HMR(LIQUID)=-1964            -1963.      5.00E+02   1.082      2.1632E-03
111 HMR(LIQUID)=-3500            -3490.      5.00E+02   10.37      2.0734E-02
112 HMR(LIQUID)=-4588            -4580.      5.00E+02   7.857      1.5714E-02
113 HMR(LIQUID)=-5239            -5234.      5.00E+02   4.551      9.1017E-03
114 HMR(LIQUID)=-5454            -5453.      5.00E+02   1.449      2.8977E-03
115 HMR(LIQUID)=-5233            -5234.      5.00E+02  -1.449     -2.8983E-03
116 HMR(LIQUID)=-4575            -4580.      5.00E+02  -5.143     -1.0286E-02
117 HMR(LIQUID)=-3481            -3490.      5.00E+02  -8.633     -1.7266E-02
118 HMR(LIQUID)=-1950            -1963.      5.00E+02  -12.92     -2.5837E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ The liquid data fitted reasonable, fix its parameters to simplify
PARROT: l-p-d liq
   ... the command in full is LIST_PHASE_DATA


 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T
PARROT: s-f-v 11-14
   ... the command in full is SET_FIX_VARIABLE
PARROT: @@ Rescale the start values of the parameters to current values
```

```
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: l-a-v
   ... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02809885E+04    2.02809885E+04    2.02809885E+04    0.00000000E+00
 V2     -2.92651699E+01   -2.92651699E+01   -2.92651699E+01    0.00000000E+00
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43675665E+04    2.43675665E+04    2.43675665E+04    0.00000000E+00
 V16    -8.56377518E+00   -8.56377518E+00   -8.56377518E+00    0.00000000E+00
 V17     3.11464876E+03    3.11464876E+03    3.11464876E+03    0.00000000E+00
 V19     2.19570764E+04    2.19570764E+04    2.19570764E+04    0.00000000E+00
 V20    -7.01093190E+00   -7.01093190E+00   -7.01093190E+00    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT:Hit RETURN to continue
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
```

```
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28

Phase region boundary   1 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary   2 at:   7.141E-01  3.000E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria

Phase region boundary   3 at:   6.817E-01  7.266E+02
 ** A2B
    BCC
 ** BCC#2

Phase region boundary   4 at:   3.625E-01  7.266E+02
 ** A2B
    BCC
Calculated.                     15  equilibria

Phase region boundary   5 at:   3.778E-01  1.185E+03
 ** LIQUID
 ** A2B
    BCC

Phase region boundary   6 at:   2.888E-01  1.185E+03
 ** LIQUID
    BCC
Calculated                     28  equilibria

Phase region boundary   7 at:   4.900E-01  1.185E+03
 ** LIQUID
    A2B
Calculated.                     33  equilibria

Phase region boundary   8 at:   6.482E-01  1.039E+03
 ** LIQUID
    A2B
 ** BCC

Phase region boundary   9 at:   7.637E-01  1.039E+03
    A2B
 ** BCC
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.259E-01  1.039E+03
    LIQUID
 ** BCC
Calculated.                      8  equilibria

Phase region boundary  11 at:   8.759E-01  1.204E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.811E-01  1.204E+03
    LIQUID
 ** FCC
Calculated                     32  equilibria

Phase region boundary  13 at:   9.361E-01  1.204E+03
    BCC
 ** FCC
Calculated                     20  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
```

```
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  26 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  29 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.435E-01  1.230E+03
 ** LIQUID
    BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.435E-01  1.230E+03
 ** LIQUID
    BCC
Calculated                     26  equilibria

Phase region boundary  33 at:   8.867E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.867E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                     29  equilibria

Phase region boundary  35 at:   6.404E-03  1.397E+03
    LIQUID
 ** BCC
Calculated                     10  equilibria

Phase region boundary  36 at:   6.404E-03  1.397E+03
    LIQUID
 ** BCC
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.295E-01  1.243E+03
    LIQUID
 ** BCC
Calculated                     22  equilibria

Phase region boundary  38 at:   2.295E-01  1.243E+03
    LIQUID
 ** BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.215E+03
    LIQUID
 ** A2B
Calculated.                     12  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.122E-01  1.215E+03
    LIQUID
 ** A2B
Calculated.                      8  equilibria
```

```
 Terminating at known equilibrium

 Phase region boundary  41 at:    9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                     19  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:    9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                     13  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                    1  seconds
POLY_3: post
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



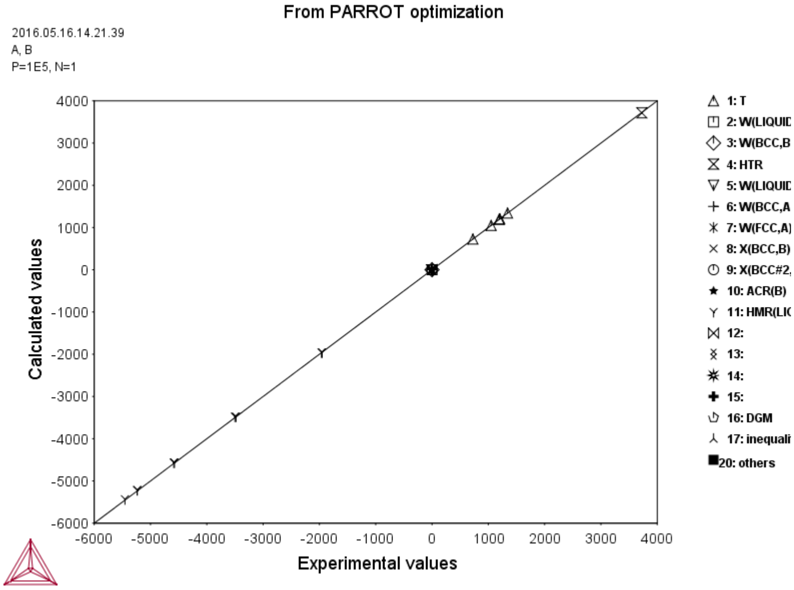
```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use     824 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88760571E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    5.88814903E-02
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    5.88785935E-02
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    5.88751225E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88749460E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88746800E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88754522E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88744378E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    7 iterations
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

  1  6.9039E-03   2  6.9039E-03   3  1.5746E-03   4  2.8286E-03   5  1.3310E-01
  6 -1.3983E-01   7 -1.4164E-03   8  7.6472E-03   9  7.6472E-03  10  1.9847E-06
 11  3.3001E-03  12  2.2286E-03  13  2.5992E-04  14  3.0133E-03  15  6.0473E-04
 16  1.1906E-03  17  1.1906E-03  18  2.3705E-04  19  1.3648E-03  20  2.3705E-04
```

```
 21  1.3648E-03  22 -2.1141E-03  23  1.7687E-03  24  3.4041E-03  25  3.3248E-04
 26 -2.5998E-03  27  3.2539E-03  28 -1.3406E-03  29  3.8359E-03  30 -1.3478E-02
 31 -3.0855E-02  32 -6.3336E-04  33  4.3684E-02  34  6.7408E-02  35  3.5765E-02
 36 -8.4872E-02  37  1.1726E-02  38 -5.6892E-02  39  2.1632E-03  40  2.0734E-02
 41  1.5714E-02  42  9.1017E-03  43  2.8977E-03  44 -2.8983E-03  45 -1.0286E-02
 46 -1.7266E-02  47 -2.5837E-02

                THE SUM OF SQUARES IS   5.88744378E-02
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use     824 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88744378E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    5.88798231E-02
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    5.88770243E-02
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    5.88744664E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88743603E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88740934E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88747821E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88738857E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    7 iterations
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

  1  6.9039E-03   2  6.9039E-03   3  1.5745E-03   4  2.7586E-03   5  1.3310E-01
  6 -1.3983E-01   7 -1.4164E-03   8  7.6472E-03   9  7.6472E-03  10 -6.7437E-05
 11  3.2926E-03  12  2.1470E-03  13  2.5560E-04  14  2.9506E-03  15  6.0313E-04
 16  1.2088E-03  17  1.2088E-03  18  1.3409E-04  19  1.4165E-03  20  1.3409E-04
 21  1.4165E-03  22 -2.1840E-03  23  1.7680E-03  24  3.3372E-03  25  3.3146E-04
 26 -2.6628E-03  27  3.2524E-03  28 -1.4140E-03  29  3.8295E-03  30 -1.3478E-02
 31 -3.0855E-02  32 -6.3336E-04  33  4.3684E-02  34  6.7408E-02  35  3.5765E-02
 36 -8.4872E-02  37  1.1726E-02  38 -5.6892E-02  39  2.1632E-03  40  2.0734E-02
 41  1.5714E-02  42  9.1017E-03  43  2.8977E-03  44 -2.8983E-03  45 -1.0286E-02
 46 -1.7266E-02  47 -2.5837E-02

                THE SUM OF SQUARES IS   5.88738857E-02
PARROT: @@ No change in the parameters, check the diagram again
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
```

```
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC
  ** BCC#2
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC
  ** BCC#2
 Calculated.                     14  equilibria

 Phase region boundary   3 at:   6.817E-01  7.266E+02
  ** A2B
     BCC
  ** BCC#2

 Phase region boundary   4 at:   3.625E-01  7.266E+02
  ** A2B
     BCC
 Calculated.                     15  equilibria

 Phase region boundary   5 at:   3.778E-01  1.185E+03
  ** LIQUID
  ** A2B
     BCC

 Phase region boundary   6 at:   2.887E-01  1.185E+03
  ** LIQUID
     BCC
 Calculated                     25  equilibria

 Phase region boundary   7 at:   4.900E-01  1.185E+03
  ** LIQUID
     A2B
 Calculated.                     33  equilibria

 Phase region boundary   8 at:   6.482E-01  1.039E+03
  ** LIQUID
     A2B
  ** BCC

 Phase region boundary   9 at:   7.637E-01  1.039E+03
     A2B
  ** BCC
 Calculated.                     10  equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   8.259E-01  1.039E+03
     LIQUID
  ** BCC
 Calculated.                      8  equilibria

 Phase region boundary  11 at:   8.758E-01  1.204E+03
     LIQUID
  ** BCC
  ** FCC

 Phase region boundary  12 at:   8.811E-01  1.204E+03
     LIQUID
  ** FCC
 Calculated                     33  equilibria

 Phase region boundary  13 at:   9.361E-01  1.204E+03
     BCC
  ** FCC
 Calculated                     18  equilibria
```

```
Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated                      10  equilibria

Phase region boundary  26 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated.                       3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated                      10  equilibria

Phase region boundary  29 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated.                       3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated.                       9  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.435E-01  1.230E+03
 ** LIQUID
    BCC
Calculated.                       4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.435E-01  1.230E+03
 ** LIQUID
    BCC
Calculated                      26  equilibria
```

```
 Phase region boundary  33 at:   8.867E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                       2  equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.867E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                      29  equilibria

 Phase region boundary  35 at:   6.404E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated                      11  equilibria

 Phase region boundary  36 at:   6.404E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated.                      13  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.295E-01  1.243E+03
     LIQUID
  ** BCC
 Calculated                      22  equilibria

 Phase region boundary  38 at:   2.295E-01  1.243E+03
     LIQUID
  ** BCC
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.215E+03
     LIQUID
  ** A2B
 Calculated.                      12  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.215E+03
     LIQUID
  ** A2B
 Calculated.                       8  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                      19  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      14  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                       1  seconds
POLY_3: post
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Turn off alternate mode and try to calculate all equilibria
PARROT: s-alt Y
   ... the command in full is SET_ALTERNATE_MODE
 Alternate calculation is on
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
```

```
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   4   1.    1184.6      LIQUID A2B BCC
   2 AINV   2   1.    1314.5      LIQUID A2B
   3 AINV   3   1.    1039.0      LIQUID A2B BCC
   4 AINV   3   1.    1204.2      LIQUID BCC FCC
   5 AINV   3   1.     726.6      A2B BCC BCC#2
   6 AINV   3   1.     726.0      BCC BCC#2
  10 ALF  < unused >  1594.0      LIQUID FCC
  11 ALF  < unused >  1548.0      LIQUID FCC
  12 ALF  < unused >  1499.0      LIQUID FCC
  13 ALF  < unused >  1438.0      LIQUID FCC
  20 ATIE   3   1.    1413.0      LIQUID FCC
  21 ATIE   3   1.    1337.0      LIQUID FCC
  22 ATIE   3   1.    1213.0      LIQUID FCC
  23 ATIE   3   1.    1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     2   1.    1773.0      LIQUID
 116 AH     2   1.    1773.0      LIQUID
 117 AH     2   1.    1773.0      LIQUID
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
ED_EXP: @@ any liquid parameters and restore those with label ALF
ED_EXP: s-we 0 100-118
   ... the command in full is SET_WEIGHT
ED_EXP: s-we 1 alf
   ... the command in full is SET_WEIGHT
 Changed weight on                      4  equilibria.
ED_EXP: s-e 1
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                      1 , label AINV
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1184.6      LIQUID A2B BCC
   2 AINV   2   1.    1314.5      LIQUID A2B
   3 AINV   2   1.    1039.0      LIQUID A2B BCC
   4 AINV   2   1.    1204.2      LIQUID BCC FCC
   5 AINV   2   1.     726.6      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    3   1.    1594.0      LIQUID FCC
  11 ALF    3   1.    1548.0      LIQUID FCC
  12 ALF    3   1.    1499.0      LIQUID FCC
  13 ALF    3   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA   < unused >  1573.0      LIQUID
 101 AA   < unused >  1573.0      LIQUID
 102 AA   < unused >  1573.0      LIQUID
 103 AA   < unused >  1573.0      LIQUID
 104 AA   < unused >  1573.0      LIQUID
 105 AA   < unused >  1573.0      LIQUID
 106 AA   < unused >  1573.0      LIQUID
 107 AA   < unused >  1573.0      LIQUID
 108 AA   < unused >  1573.0      LIQUID
 110 AH   < unused >  1773.0      LIQUID
 111 AH   < unused >  1773.0      LIQUID
 112 AH   < unused >  1773.0      LIQUID
 113 AH   < unused >  1773.0      LIQUID
 114 AH   < unused >  1773.0      LIQUID
 115 AH   < unused >  1773.0      LIQUID
 116 AH   < unused >  1773.0      LIQUID
 117 AH   < unused >  1773.0      LIQUID
 118 AH   < unused >  1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:40




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:    0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =    0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03
```

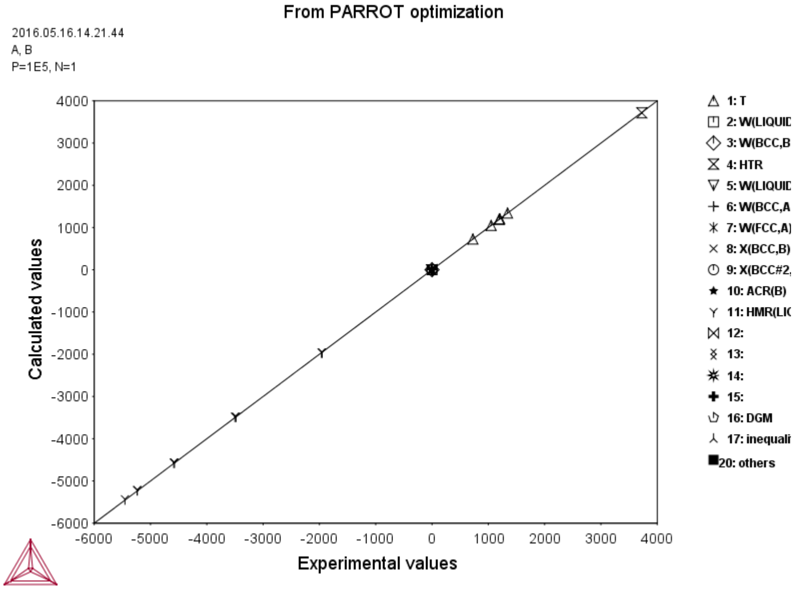
```
 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02809885E+04    2.02809885E+04    2.02809885E+04    7.39143651E-02
 V2     -2.92651699E+01   -2.92651699E+01   -2.92651699E+01    3.41787474E-01
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43700033E+04    2.43700033E+04    2.43700033E+04    6.09487672E-01
 V16    -8.56548802E+00   -8.56463156E+00   -8.56463156E+00    2.04922287E+00
 V17     3.11527172E+03    3.11496022E+03    3.11496022E+03    1.45833479E+00
 V19     2.19570764E+04    2.19570764E+04    2.19570764E+04    4.63522316E+00
 V20    -7.01233415E+00   -7.01163299E+00   -7.01163299E+00    1.12486774E+01

 NUMBER OF OPTIMIZING VARIABLES :    7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.88744378E-02 TO   8.99443380E+00
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   4.08837900E-01


 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0280989E+04
   4 V2        48000000 -2.9265170E+01
  13 V11       48000000 -2.1810205E+04
  14 V12       48000000  1.5161309E+01
  17 V15       48000000  2.4370003E+04
  18 V16       48000000 -8.5654880E+00
  19 V17       48000000  3.1152717E+03
  21 V19       48000000  2.1957076E+04
  22 V20       48000000 -7.0123342E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                         1185.      10.0      -8.445     -0.8445
1 W(LIQUID,B)=0.408             0.4163      2.00E-02  8.3025E-03  0.4151
1 W(BCC,B)=0.13                 0.1322      2.00E-02  2.2006E-03  0.1100
2 T=1341                         1315.      10.0      -26.49      -2.649
2 HTR=3727                       3726.      5.00E+02 -0.7083     -1.4167E-03
3 T=1049                         1039.      10.0      -10.03      -1.003
3 W(LIQUID,A)=0.27              0.2735      2.00E-02  3.4728E-03  0.1736
3 W(BCC,A)=9.3E-2               9.3787E-02  2.00E-02  7.8737E-04  3.9368E-02
4 T=1203                         1204.      10.0       1.179      0.1179
4 W(LIQUID,A)=0.19              0.1890      2.00E-02 -9.8135E-04 -4.9067E-02
4 W(BCC,A)=6.9E-2               6.8455E-02  2.00E-02 -5.4510E-04 -2.7255E-02
4 W(FCC,A)=6E-2                 5.9376E-02  2.00E-02 -6.2387E-04 -3.1194E-02
5 T=726                          726.6      10.0      0.6276      6.2757E-02
5 X(BCC,B)=3.7E-2               3.7255E-02  2.00E-02  2.5471E-04  1.2736E-02
5 X(BCC#2,A)=0.114              0.1144      2.00E-02  4.0100E-04  2.0050E-02
6 X(BCC,B)=3.7E-2               3.7078E-02  2.00E-02  7.8113E-05  3.9056E-03
6 X(BCC#2,A)=0.114              0.1140      2.00E-02 -3.4068E-05 -1.7034E-03
10 W(LIQUID,A)=2E-2             1.9384E-02  2.00E-02 -6.1575E-04 -3.0788E-02
11 W(LIQUID,A)=4.2E-2           4.1484E-02  2.00E-02 -5.1605E-04 -2.5802E-02
12 W(LIQUID,A)=6.5E-2           6.4387E-02  2.00E-02 -6.1266E-04 -3.0633E-02
13 W(LIQUID,A)=9.3E-2           9.2002E-02  2.00E-02 -9.9776E-04 -4.9888E-02
20 W(LIQUID,A)=0.104            0.1030      2.00E-02 -9.6497E-04 -4.8249E-02
20 W(FCC,A)=3.8E-2              3.7713E-02  2.00E-02 -2.8716E-04 -1.4358E-02
21 W(LIQUID,A)=0.136            0.1356      2.00E-02 -4.2474E-04 -2.1237E-02
21 W(FCC,A)=4.7E-2              4.6609E-02  2.00E-02 -3.9077E-04 -1.9538E-02
22 W(LIQUID,A)=0.187            0.1856      2.00E-02 -1.4041E-03 -7.0205E-02
22 W(FCC,A)=5.9E-2              5.8614E-02  2.00E-02 -3.8608E-04 -1.9304E-02
23 W(LIQUID,A)=0.245            0.2434      2.00E-02 -1.5869E-03 -7.9344E-02
23 W(BCC,A)=8.5E-2              8.4361E-02  2.00E-02 -6.3920E-04 -3.1960E-02


PARROT:
```

```
PARROT:Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for equilibrium 4
PARROT: @@ It can be on the wrong side, at high A instead of high B. Try to correct
PARROT: @@ that in the edit module.
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                      4 , label AINV
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.179217/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    13 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC=1     FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1204.18 K (   931.03 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.30210E+02
 Total Gibbs energy -9.82098E+03,  Enthalpy  1.98581E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.5966E-01  1.0132E-01 3.8855E-01 -9.4648E+03 SER
 B                       2.3403E+00  8.9868E-01 8.5841E-01 -1.5286E+03 SER

 FCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5911E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.40624E-01  A  5.93761E-02

 BCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5344E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.31545E-01  A  6.84549E-02

 LIQUID                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.8955E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.10981E-01  A  1.89019E-01

 EXPERIMENT T=1203:DT  $1204.18:10  NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX  $0.189019:2E-2  NO=2
 EXPERIMENT W(BCC,A)=6.9E-2:DX  $6.84549E-2:2E-2  NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX  $5.93761E-2:2E-2  NO=4
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ The error is still there, calculate the phase diagram!!!
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.
```

```
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC
  ** BCC#2
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC
  ** BCC#2
 Calculated.                     14  equilibria

 Phase region boundary   3 at:   6.817E-01  7.266E+02
  ** A2B
     BCC
  ** BCC#2

 Phase region boundary   4 at:   3.625E-01  7.266E+02
  ** A2B
     BCC
 Calculated.                     15  equilibria

 Phase region boundary   5 at:   3.778E-01  1.185E+03
  ** LIQUID
  ** A2B
     BCC

 Phase region boundary   6 at:   2.887E-01  1.185E+03
  ** LIQUID
     BCC
 Calculated                     25  equilibria

 Phase region boundary   7 at:   4.900E-01  1.185E+03
  ** LIQUID
     A2B
 Calculated.                     33  equilibria

 Phase region boundary   8 at:   6.482E-01  1.039E+03
  ** LIQUID
     A2B
  ** BCC

 Phase region boundary   9 at:   7.637E-01  1.039E+03
     A2B
  ** BCC
 Calculated.                     10  equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   8.259E-01  1.039E+03
     LIQUID
  ** BCC
 Calculated.                      8  equilibria

 Phase region boundary  11 at:   8.758E-01  1.204E+03
     LIQUID
  ** BCC
  ** FCC

 Phase region boundary  12 at:   8.811E-01  1.204E+03
     LIQUID
  ** FCC
 Calculated                     33  equilibria

 Phase region boundary  13 at:   9.361E-01  1.204E+03
     BCC
  ** FCC
```

```
Calculated                     18  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  26 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.646E-01  7.700E+02
 ** A2B
    BCC
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  29 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.909E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.435E-01  1.230E+03
 ** LIQUID
    BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.435E-01  1.230E+03
 ** LIQUID
    BCC
```

```
 Calculated                     26  equilibria

 Phase region boundary  33 at:   8.867E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                      2  equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.867E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                     29  equilibria

 Phase region boundary  35 at:   6.404E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated                     11  equilibria

 Phase region boundary  36 at:   6.404E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated.                     13  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.295E-01  1.243E+03
     LIQUID
  ** BCC
 Calculated                     22  equilibria

 Phase region boundary  38 at:   2.295E-01  1.243E+03
     LIQUID
  ** BCC
 Calculated.                      4  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.215E+03
     LIQUID
  ** A2B
 Calculated.                     12  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.215E+03
     LIQUID
  ** A2B
 Calculated.                      8  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                     19  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                     14  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                      1  seconds
POLY_3: post
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: ed
```

```
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: s-we 0 4
   ... the command in full is SET_WEIGHT
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use      25 experiments, maximum is        2000
 Use     494 real workspace, maximum is    50000
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:45




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =    0    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02809885E+04    2.02809885E+04    2.02809885E+04    7.39143651E-02
 V2     -2.92651699E+01   -2.92651699E+01   -2.92651699E+01    3.41787474E-01
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43700033E+04    2.43700033E+04    2.43700033E+04    6.09487672E-01
 V16    -8.56548802E+00   -8.56463156E+00   -8.56463156E+00    2.04922287E+00
 V17     3.11527172E+03    3.11496022E+03    3.11496022E+03    1.45833479E+00
 V19     2.19570764E+04    2.19570764E+04    2.19570764E+04    4.63522316E+00
 V20    -7.01233415E+00   -7.01163299E+00   -7.01163299E+00    1.12486774E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.88744378E-02 TO   8.97640476E+00
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   4.98689154E-01


 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0280989E+04
   4 V2        48000000 -2.9265170E+01
  13 V11       48000000 -2.1810205E+04
  14 V12       48000000  1.5161309E+01
  17 V15       48000000  2.4370003E+04
  18 V16       48000000 -8.5654880E+00
  19 V17       48000000  3.1152717E+03
  21 V19       48000000  2.1957076E+04
  22 V20       48000000 -7.0123342E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T


$ ======  BLOCK NUMBER  1
```

```
 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                         1185.      10.0      -8.445     -0.8445
1 W(LIQUID,B)=0.408             0.4163     2.00E-02  8.3025E-03  0.4151
1 W(BCC,B)=0.13                 0.1322     2.00E-02  2.2006E-03  0.1100
2 T=1341                         1315.      10.0      -26.49      -2.649
2 HTR=3727                       3726.     5.00E+02 -0.7083     -1.4167E-03
3 T=1049                         1039.      10.0      -10.03      -1.003
3 W(LIQUID,A)=0.27              0.2735     2.00E-02  3.4728E-03  0.1736
3 W(BCC,A)=9.3E-2               9.3787E-02  2.00E-02  7.8737E-04  3.9368E-02
5 T=726                          726.6      10.0      0.6276      6.2757E-02
5 X(BCC,B)=3.7E-2               3.7255E-02  2.00E-02  2.5471E-04  1.2736E-02
5 X(BCC#2,A)=0.114              0.1144     2.00E-02  4.0100E-04  2.0050E-02
6 X(BCC,B)=3.7E-2               3.7078E-02  2.00E-02  7.8113E-05  3.9056E-03
6 X(BCC#2,A)=0.114              0.1140     2.00E-02 -3.4068E-05 -1.7034E-03
10 W(LIQUID,A)=2E-2             1.9384E-02  2.00E-02 -6.1575E-04 -3.0788E-02
11 W(LIQUID,A)=4.2E-2           4.1484E-02  2.00E-02 -5.1605E-04 -2.5802E-02
12 W(LIQUID,A)=6.5E-2           6.4387E-02  2.00E-02 -6.1266E-04 -3.0633E-02
13 W(LIQUID,A)=9.3E-2           9.2002E-02  2.00E-02 -9.9776E-04 -4.9888E-02
20 W(LIQUID,A)=0.104            0.1030     2.00E-02 -9.6497E-04 -4.8249E-02
20 W(FCC,A)=3.8E-2              3.7713E-02  2.00E-02 -2.8716E-04 -1.4358E-02
21 W(LIQUID,A)=0.136            0.1356     2.00E-02 -4.2474E-04 -2.1237E-02
21 W(FCC,A)=4.7E-2              4.6609E-02  2.00E-02 -3.9077E-04 -1.9538E-02
22 W(LIQUID,A)=0.187            0.1856     2.00E-02 -1.4041E-03 -7.0205E-02
22 W(FCC,A)=5.9E-2              5.8614E-02  2.00E-02 -3.8608E-04 -1.9304E-02
23 W(LIQUID,A)=0.245            0.2434     2.00E-02 -1.5869E-03 -7.9344E-02
23 W(BCC,A)=8.5E-2              8.4361E-02  2.00E-02 -6.3920E-04 -3.1960E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use      25 experiments, maximum is        2000
 Use     494 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


     AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    8.97640476E+00
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

     AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    9.13900120E+00
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

     AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    8.68324796E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

     AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    8.69026383E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

     AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    8.68061561E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0002E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    8.68025225E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0002E+00   5  1.0002E+00
  6  1.0000E+00   7  1.0001E+00

     AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    8.68061354E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0002E+00   5  1.0002E+00
  6  1.0001E+00   7  1.0001E+00

     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    8.68010001E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0002E+00   5  1.0002E+00
  6  1.0000E+00   7  1.0002E+00

     AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    4.74733287E-01
  1  9.9763E-01   2  1.0044E+00   3  9.9990E-01   4  1.0002E+00   5  1.0002E+00
  6  9.9999E-01   7  1.0002E+00

     AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    3.94612071E-01
  1  9.9883E-01   2  1.0048E+00   3  9.9988E-01   4  1.0031E+00   5  1.0015E+00
  6  1.0010E+00   7  1.0037E+00

     AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    3.39925250E-01
  1  9.9933E-01   2  1.0054E+00   3  1.0002E+00   4  1.0049E+00   5  1.0023E+00
  6  1.0045E+00   7  1.0127E+00

     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    2.09925807E-01
  1  1.0023E+00   2  1.0068E+00   3  1.0020E+00   4  1.0149E+00   5  1.0070E+00
  6  9.9722E-01   7  9.9852E-01

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27916004E-01
  1  1.0072E+00   2  1.0096E+00   3  1.0064E+00   4  1.0333E+00   5  1.0153E+00
  6  1.0040E+00   7  1.0210E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   12 iterations
  1  1.0072E+00   2  1.0096E+00   3  1.0064E+00   4  1.0333E+00   5  1.0153E+00
  6  1.0040E+00   7  1.0210E+00

  1 -1.2012E-01   2  1.6807E-02   3  7.7726E-02   4  7.5285E-02   5 -9.8949E-02
  6 -1.6451E-01   7  5.6332E-02   8  1.1680E-01   9 -1.5429E-01  10 -1.7636E-02
 11  3.4908E-02  12  4.0882E-03  13  8.9192E-02  14 -2.2047E-02  15 -9.2884E-03
 16 -8.1454E-03  17 -2.2546E-02  18 -1.9582E-02  19  1.7801E-02  20  9.6277E-03
 21  1.8367E-02  22 -3.9899E-02  23  2.5880E-02  24  9.1761E-03  25  9.9469E-02

              THE SUM OF SQUARES IS   1.27916004E-01
PARROT: cont 30
   ... the command in full is CONTINUE_OPTIMIZATION

 It is safe to CONTINUE only after TOO MANY ITERATIONS
 and no change in variables and experiments ...
 Now anything can happen ...

PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
```

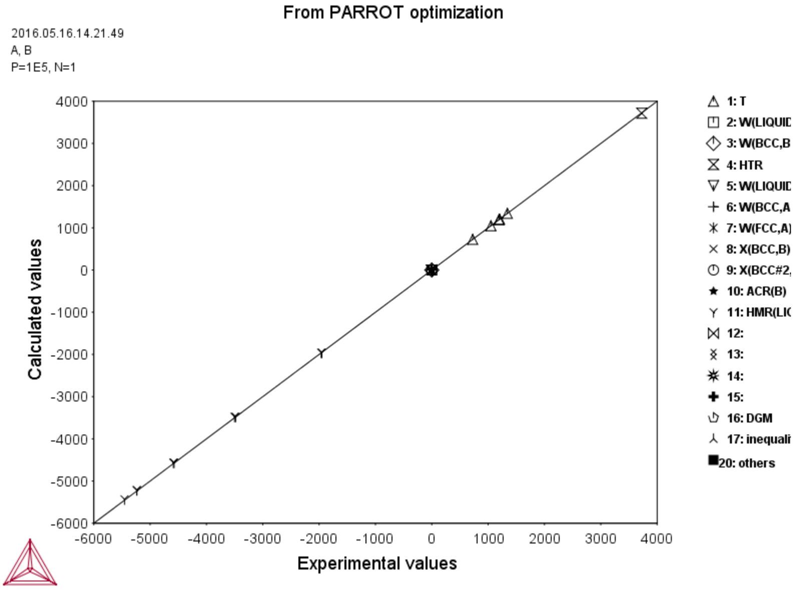
```
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:45



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  13


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04272876E+04    2.02809885E+04    2.02809885E+04    2.59209705E-02
 V2     -2.95468613E+01   -2.92651699E+01   -2.92651699E+01    1.40177728E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.45250655E+04    2.43700033E+04    2.43700033E+04    9.62418602E-02
 V16    -8.85015072E+00   -8.56463156E+00   -8.56463156E+00    2.78844062E-01
 V17     3.16252983E+03    3.11496022E+03    3.11496022E+03    2.49147755E-01
 V19     2.20441098E+04    2.19570764E+04    2.19570764E+04    6.73748360E-01
 V20    -7.15892220E+00   -7.01163299E+00   -7.01163299E+00    1.60351723E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.97640476E+00 TO   1.27916004E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   7.10644464E-03


 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0427288E+04
   4 V2        48000000 -2.9546861E+01
  13 V11       48000000 -2.1810205E+04
  14 V12       48000000  1.5161309E+01
  17 V15       48000000  2.4525066E+04
  18 V16       48000000 -8.8501507E+00
  19 V17       48000000  3.1625298E+03
  21 V19       48000000  2.2044110E+04
  22 V20       48000000 -7.1589222E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                         1192.      10.0      -1.201     -0.1201
1 W(LIQUID,B)=0.408             0.4083      2.00E-02  3.3615E-04  1.6807E-02
1 W(BCC,B)=0.13                 0.1316      2.00E-02  1.5545E-03  7.7726E-02
2 T=1341                         1342.      10.0      0.7529      7.5285E-02
2 HTR=3727                       3678.      5.00E+02  -49.47     -9.8949E-02
3 T=1049                         1047.      10.0      -1.645     -0.1645
3 W(LIQUID,A)=0.27              0.2711      2.00E-02  1.1266E-03  5.6332E-02
3 W(BCC,A)=9.3E-2               9.5336E-02  2.00E-02  2.3361E-03  0.1168
5 T=726                          724.5      10.0      -1.543     -0.1543
5 X(BCC,B)=3.7E-2               3.6647E-02  2.00E-02 -3.5272E-04 -1.7636E-02
5 X(BCC#2,A)=0.114              0.1147      2.00E-02  6.9816E-04  3.4908E-02
6 X(BCC,B)=3.7E-2               3.7082E-02  2.00E-02  8.1763E-05  4.0882E-03
6 X(BCC#2,A)=0.114              0.1158      2.00E-02  1.7838E-03  8.9192E-02
```

```
10 W(LIQUID,A)=2E-2              1.9559E-02  2.00E-02 -4.4094E-04 -2.2047E-02
11 W(LIQUID,A)=4.2E-2            4.1814E-02  2.00E-02 -1.8577E-04 -9.2884E-03
12 W(LIQUID,A)=6.5E-2            6.4837E-02  2.00E-02 -1.6291E-04 -8.1454E-03
13 W(LIQUID,A)=9.3E-2            9.2549E-02  2.00E-02 -4.5092E-04 -2.2546E-02
20 W(LIQUID,A)=0.104             0.1036      2.00E-02 -3.9164E-04 -1.9582E-02
20 W(FCC,A)=3.8E-2               3.8356E-02  2.00E-02  3.5602E-04  1.7801E-02
21 W(LIQUID,A)=0.136             0.1362      2.00E-02  1.9255E-04  9.6277E-03
21 W(FCC,A)=4.7E-2               4.7367E-02  2.00E-02  3.6734E-04  1.8367E-02
22 W(LIQUID,A)=0.187             0.1862      2.00E-02 -7.9799E-04 -3.9899E-02
22 W(FCC,A)=5.9E-2               5.9518E-02  2.00E-02  5.1760E-04  2.5880E-02
23 W(LIQUID,A)=0.245             0.2452      2.00E-02  1.8352E-04  9.1761E-03
23 W(BCC,A)=8.5E-2               8.6989E-02  2.00E-02  1.9894E-03  9.9469E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Optimization converged, try to add equilibrium 4 again
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                      4 , label AINV
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.179217/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    13 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC=1     FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1211.83 K (   938.68 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.30242E+02
 Total Gibbs energy -1.00413E+04,  Enthalpy  1.99592E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 A                        6.5860E-01  1.0113E-01 3.8288E-01 -9.6731E+03 SER
 B                        2.3414E+00  8.9887E-01 8.5591E-01 -1.5677E+03 SER

 FCC                          Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5896E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.40380E-01  A  5.96204E-02

 BCC                          Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5283E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.30563E-01  A  6.94370E-02

 LIQUID                       Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.9063E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.13344E-01  A  1.86656E-01

 SET_WEIGHT 0,,,
 EXPERIMENT T=1203:DT
 EXPERIMENT W(LIQUID,A)=0.19:DX
 EXPERIMENT W(BCC,A)=6.9E-2:DX
 EXPERIMENT W(FCC,A)=6E-2:DX
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
```

```
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC
  ** BCC#2
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC
  ** BCC#2
 Calculated.                      14  equilibria

 Phase region boundary   3 at:   6.813E-01  7.245E+02
  ** A2B
     BCC
  ** BCC#2

 Phase region boundary   4 at:   3.620E-01  7.245E+02
  ** A2B
     BCC
 Calculated.                      15  equilibria

 Phase region boundary   5 at:   3.775E-01  1.192E+03
  ** LIQUID
  ** A2B
     BCC

 Phase region boundary   6 at:   2.837E-01  1.192E+03
  ** LIQUID
     BCC
 Calculated                      24  equilibria

 Phase region boundary   7 at:   4.865E-01  1.192E+03
  ** LIQUID
     A2B
 Calculated.                      33  equilibria

 Phase region boundary   8 at:   6.495E-01  1.047E+03
  ** LIQUID
     A2B
  ** BCC

 Phase region boundary   9 at:   7.626E-01  1.047E+03
     A2B
  ** BCC
 Calculated.                      11  equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   8.259E-01  1.047E+03
     LIQUID
  ** BCC
 Calculated.                       9  equilibria
```

```
Phase region boundary  11 at:   8.763E-01  1.212E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.820E-01  1.212E+03
    LIQUID
 ** FCC
Calculated                     35  equilibria

Phase region boundary  13 at:   9.355E-01  1.212E+03
    BCC
 ** FCC
Calculated                     24  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.642E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  26 at:   3.642E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.642E-01  7.700E+02
 ** A2B
    BCC
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.905E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  29 at:   7.905E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.905E-01  7.700E+02
```

```
  ** A2B
     BCC
 Calculated.                       9  equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.451E-01  1.230E+03
  ** LIQUID
     BCC
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.451E-01  1.230E+03
  ** LIQUID
     BCC
 Calculated                      26  equilibria

 Phase region boundary  33 at:   8.859E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                       2  equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.859E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                      29  equilibria

 Phase region boundary  35 at:   6.428E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated                        8  equilibria

 Phase region boundary  36 at:   6.428E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated.                      13  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.303E-01  1.244E+03
     LIQUID
  ** BCC
 Calculated                      22  equilibria

 Phase region boundary  38 at:   2.303E-01  1.244E+03
     LIQUID
  ** BCC
 Calculated.                       4  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.239E+03
     LIQUID
  ** A2B
 Calculated.                      14  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.239E+03
     LIQUID
  ** A2B
 Calculated.                       8  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                      19  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                        9  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                       1  seconds
POLY_3: post
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
```

```
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ Sometimes a very strange shape of the fcc phase here and no
POST: @@ equilibrium between liq, fcc and bcc at high B content.
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:50




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  13


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04272876E+04    2.02809885E+04    2.02809885E+04    2.59209705E-02
 V2     -2.95468613E+01   -2.92651699E+01   -2.92651699E+01    1.40177728E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.45250655E+04    2.43700033E+04    2.43700033E+04    9.62418602E-02
 V16    -8.85015072E+00   -8.56463156E+00   -8.56463156E+00    2.78844062E-01
 V17     3.16252983E+03    3.11496022E+03    3.11496022E+03    2.49147755E-01
 V19     2.20441098E+04    2.19570764E+04    2.19570764E+04    6.73748360E-01
 V20    -7.15892220E+00   -7.01163299E+00   -7.01163299E+00    1.60351723E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.97640476E+00 TO   1.27916004E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   7.10644464E-03


 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0427288E+04
   4 V2        48000000 -2.9546861E+01
  13 V11       48000000 -2.1810205E+04
  14 V12       48000000  1.5161309E+01
  17 V15       48000000  2.4525066E+04
  18 V16       48000000 -8.8501507E+00
  19 V17       48000000  3.1625298E+03
  21 V19       48000000  2.2044110E+04
  22 V20       48000000 -7.1589222E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T


$ ======  BLOCK NUMBER  1
```

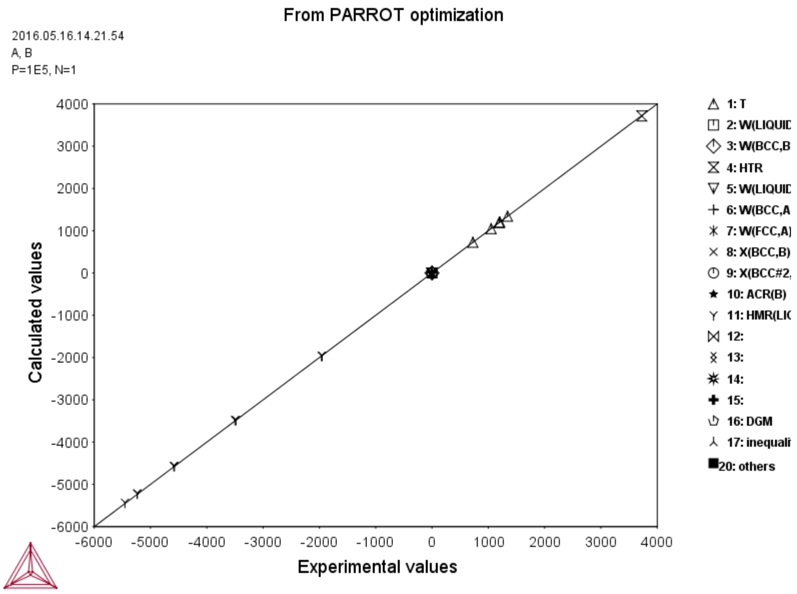
```
 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.      10.0      -1.201     -0.1201
1 W(LIQUID,B)=0.408              0.4083     2.00E-02  3.3615E-04  1.6807E-02
1 W(BCC,B)=0.13                  0.1316     2.00E-02  1.5545E-03  7.7726E-02
2 T=1341                          1342.      10.0      0.7529      7.5285E-02
2 HTR=3727                        3678.      5.00E+02  -49.47     -9.8949E-02
3 T=1049                          1047.      10.0      -1.645     -0.1645
3 W(LIQUID,A)=0.27               0.2711     2.00E-02  1.1266E-03  5.6332E-02
3 W(BCC,A)=9.3E-2                9.5336E-02  2.00E-02  2.3361E-03  0.1168
5 T=726                           724.5      10.0      -1.543     -0.1543
5 X(BCC,B)=3.7E-2                3.6647E-02  2.00E-02 -3.5272E-04 -1.7636E-02
5 X(BCC#2,A)=0.114               0.1147     2.00E-02  6.9816E-04  3.4908E-02
6 X(BCC,B)=3.7E-2                3.7082E-02  2.00E-02  8.1763E-05  4.0882E-03
6 X(BCC#2,A)=0.114               0.1158     2.00E-02  1.7838E-03  8.9192E-02
10 W(LIQUID,A)=2E-2              1.9559E-02  2.00E-02 -4.4094E-04 -2.2047E-02
11 W(LIQUID,A)=4.2E-2            4.1814E-02  2.00E-02 -1.8577E-04 -9.2884E-03
12 W(LIQUID,A)=6.5E-2            6.4837E-02  2.00E-02 -1.6291E-04 -8.1454E-03
13 W(LIQUID,A)=9.3E-2            9.2549E-02  2.00E-02 -4.5092E-04 -2.2546E-02
20 W(LIQUID,A)=0.104             0.1036     2.00E-02 -3.9164E-04 -1.9582E-02
20 W(FCC,A)=3.8E-2               3.8356E-02  2.00E-02  3.5602E-04  1.7801E-02
21 W(LIQUID,A)=0.136             0.1362     2.00E-02  1.9255E-04  9.6277E-03
21 W(FCC,A)=4.7E-2               4.7367E-02  2.00E-02  3.6734E-04  1.8367E-02
22 W(LIQUID,A)=0.187             0.1862     2.00E-02 -7.9799E-04 -3.9899E-02
22 W(FCC,A)=5.9E-2               5.9518E-02  2.00E-02  5.1760E-04  2.5880E-02
23 W(LIQUID,A)=0.245             0.2452     2.00E-02  1.8352E-04  9.1761E-03
23 W(BCC,A)=8.5E-2               8.6989E-02  2.00E-02  1.9894E-03  9.9469E-02


PARROT:
PARROT: @@ Note that all other experiments are well fitted!
PARROT: @@ Try to improve by optimizing a little more !!!
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use      25 experiments, maximum is        2000
 Use     494 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE     0 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27916004E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE     1 ST ITERATION WE HAVE THE SUM OF SQUARES    1.27932261E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE     2 ND ITERATION WE HAVE THE SUM OF SQUARES    1.32349433E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE     3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.27975279E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE     4 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27918247E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE     5 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27915991E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE     6 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27919898E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE     7 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27914900E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE     8 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27686419E-01
  1  1.0000E+00   2  9.9998E-01   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0002E+00

      AT THE     9 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27670632E-01
  1  9.9993E-01   2  9.9993E-01   3  9.9998E-01   4  1.0000E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0002E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED     9 iterations
  1  9.9993E-01   2  9.9993E-01   3  9.9998E-01   4  1.0000E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0002E+00

  1 -1.2292E-01   2  1.8762E-02   3  7.8915E-02   4  6.1120E-02   5 -9.7983E-02
  6 -1.6559E-01   7  5.7097E-02   8  1.1773E-01   9 -1.5386E-01  10 -1.7437E-02
 11  3.6109E-02  12  4.2281E-03  13  9.0250E-02  14 -2.1977E-02  15 -9.1582E-03
 16 -7.9707E-03  17 -2.2338E-02  18 -1.9366E-02  19  1.8043E-02  20  9.8524E-03
 21  1.8643E-02  22 -3.9695E-02  23  2.6185E-02  24  9.6601E-03  25  1.0017E-01

                THE SUM OF SQUARES IS    1.27670632E-01
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


            ===================================================
            OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:50




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  10


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30    DMAX =  1.00000000E+02    H =  1.00000000E-04
```

```
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04258378E+04    2.04272876E+04    2.04272876E+04    2.56056900E-02
 V2     -2.95449125E+01   -2.95468613E+01   -2.95468613E+01    1.38446508E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.45244730E+04    2.45250655E+04    2.45250655E+04    9.63618791E-02
 V16    -8.85034461E+00   -8.85015072E+00   -8.85015072E+00    2.70402366E-01
 V17     3.16285525E+03    3.16252983E+03    3.16252983E+03    2.49505586E-01
 V19     2.20452445E+04    2.20441098E+04    2.20441098E+04    6.66481224E-01
 V20    -7.16035825E+00   -7.15892220E+00   -7.15892220E+00    1.56212011E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.27916004E-01 TO   1.27670632E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   7.09281289E-03


 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0425838E+04
   4 V2        48000000 -2.9544913E+01
  13 V11       48000000 -2.1810205E+04
  14 V12       48000000  1.5161309E+01
  17 V15       48000000  2.4524473E+04
  18 V16       48000000 -8.8503446E+00
  19 V17       48000000  3.1628552E+03
  21 V19       48000000  2.2045244E+04
  22 V20       48000000 -7.1603583E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.      10.0      -1.229     -0.1229
1 W(LIQUID,B)=0.408              0.4084      2.00E-02  3.7523E-04  1.8762E-02
1 W(BCC,B)=0.13                  0.1316      2.00E-02  1.5783E-03  7.8915E-02
2 T=1341                          1342.      10.0      0.6112      6.1120E-02
2 HTR=3727                        3678.      5.00E+02  -48.99     -9.7983E-02
3 T=1049                          1047.      10.0      -1.656     -0.1656
3 W(LIQUID,A)=0.27               0.2711      2.00E-02  1.1419E-03  5.7097E-02
3 W(BCC,A)=9.3E-2                9.5355E-02  2.00E-02  2.3545E-03  0.1177
5 T=726                           724.5      10.0      -1.539     -0.1539
5 X(BCC,B)=3.7E-2                3.6651E-02  2.00E-02 -3.4874E-04 -1.7437E-02
5 X(BCC#2,A)=0.114               0.1147      2.00E-02  7.2219E-04  3.6109E-02
6 X(BCC,B)=3.7E-2                3.7085E-02  2.00E-02  8.4561E-05  4.2281E-03
6 X(BCC#2,A)=0.114               0.1158      2.00E-02  1.8050E-03  9.0250E-02
10 W(LIQUID,A)=2E-2              1.9560E-02  2.00E-02 -4.3955E-04 -2.1977E-02
11 W(LIQUID,A)=4.2E-2            4.1817E-02  2.00E-02 -1.8316E-04 -9.1582E-03
12 W(LIQUID,A)=6.5E-2            6.4841E-02  2.00E-02 -1.5941E-04 -7.9707E-03
13 W(LIQUID,A)=9.3E-2            9.2553E-02  2.00E-02 -4.4677E-04 -2.2338E-02
20 W(LIQUID,A)=0.104             0.1036      2.00E-02 -3.8733E-04 -1.9366E-02
20 W(FCC,A)=3.8E-2               3.8361E-02  2.00E-02  3.6086E-04  1.8043E-02
21 W(LIQUID,A)=0.136             0.1362      2.00E-02  1.9705E-04  9.8524E-03
21 W(FCC,A)=4.7E-2               4.7373E-02  2.00E-02  3.7286E-04  1.8643E-02
22 W(LIQUID,A)=0.187             0.1862      2.00E-02 -7.9389E-04 -3.9695E-02
22 W(FCC,A)=5.9E-2               5.9524E-02  2.00E-02  5.2371E-04  2.6185E-02
23 W(LIQUID,A)=0.245             0.2452      2.00E-02  1.9320E-04  9.6601E-03
23 W(BCC,A)=8.5E-2               8.7003E-02  2.00E-02  2.0035E-03  0.1002


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram again
```

```
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC
  ** BCC#2
 Calculated..                      2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC
  ** BCC#2
 Calculated.                     14  equilibria

 Phase region boundary   3 at:   6.813E-01  7.245E+02
  ** A2B
     BCC
  ** BCC#2

 Phase region boundary   4 at:   3.620E-01  7.245E+02
  ** A2B
```

```
    BCC
Calculated.                      15  equilibria

Phase region boundary   5 at:   3.775E-01  1.192E+03
 ** LIQUID
 ** A2B
    BCC

Phase region boundary   6 at:   2.837E-01  1.192E+03
 ** LIQUID
    BCC
Calculated                      26  equilibria

Phase region boundary   7 at:   4.865E-01  1.192E+03
 ** LIQUID
    A2B
Calculated.                      33  equilibria

Phase region boundary   8 at:   6.495E-01  1.047E+03
 ** LIQUID
    A2B
 ** BCC

Phase region boundary   9 at:   7.626E-01  1.047E+03
    A2B
 ** BCC
Calculated.                      11  equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.258E-01  1.047E+03
    LIQUID
 ** BCC
Calculated.                       9  equilibria

Phase region boundary  11 at:   8.763E-01  1.212E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.820E-01  1.212E+03
    LIQUID
 ** FCC
Calculated                      31  equilibria

Phase region boundary  13 at:   9.355E-01  1.212E+03
    BCC
 ** FCC
Calculated                      23  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
```

```
     BCC#2
 Calculated.                       13  equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   3.642E-01  7.700E+02
  ** A2B
     BCC
 Calculated                       10  equilibria

 Phase region boundary  26 at:   3.642E-01  7.700E+02
  ** A2B
     BCC
 Calculated.                        3  equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   3.642E-01  7.700E+02
  ** A2B
     BCC
 Calculated.                       14  equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.905E-01  7.700E+02
  ** A2B
     BCC
 Calculated                       10  equilibria

 Phase region boundary  29 at:   7.905E-01  7.700E+02
  ** A2B
     BCC
 Calculated.                        3  equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.905E-01  7.700E+02
  ** A2B
     BCC
 Calculated.                        9  equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.451E-01  1.230E+03
  ** LIQUID
     BCC
 Calculated.                        4  equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.451E-01  1.230E+03
  ** LIQUID
     BCC
 Calculated                       26  equilibria

 Phase region boundary  33 at:   8.859E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                        2  equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.859E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                       29  equilibria

 Phase region boundary  35 at:   6.428E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated                        9  equilibria

 Phase region boundary  36 at:   6.428E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated.                       13  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.303E-01  1.244E+03
     LIQUID
  ** BCC
 Calculated                       21  equilibria

 Phase region boundary  38 at:   2.303E-01  1.244E+03
     LIQUID
  ** BCC
 Calculated.                        4  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.239E+03
     LIQUID
  ** A2B
 Calculated.                       14  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.239E+03
     LIQUID
  ** A2B
 Calculated.                        8  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                       19  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                       10  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                       1  seconds
POLY_3: post
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid at high B
PARROT: @@ restore equilibrium 4 on the POP file
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                      4 , label AINV
ED_EXP: s-we 1
   ... the command in full is SET_WEIGHT
Equilibria (range) or label(s) /PRESENT/: PRESENT
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.179217/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    13 ITS,   CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC=1     FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1211.86 K (   938.71 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.30242E+02
 Total Gibbs energy -1.00423E+04,  Enthalpy  1.99596E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.5861E-01  1.0114E-01 3.8286E-01 -9.6738E+03 SER
 B                       2.3414E+00  8.9886E-01 8.5590E-01 -1.5679E+03 SER

 FCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5895E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.40376E-01  A  5.96239E-02

 BCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5283E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.30557E-01  A  6.94426E-02

 LIQUID                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.9063E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.13351E-01  A  1.86649E-01

 EXPERIMENT T=1203:DT  $1211.86:10  NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX  $0.186649:2E-2  NO=2
 EXPERIMENT W(BCC,A)=6.9E-2:DX  $6.94426E-2:2E-2  NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX  $5.96239E-2:2E-2  NO=4
ED_EXP: @@ Now equilibrium 4 is on the high B side
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
```

```
ED_EXP: ba
   ... the command in full is BACK
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:55




 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =    0    DMAX =  1.00000000E+02    H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04258378E+04    2.04258378E+04    2.04258378E+04    0.00000000E+00
 V2     -2.95449125E+01   -2.95449125E+01   -2.95449125E+01    0.00000000E+00
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.45244730E+04    2.45244730E+04    2.45244730E+04    0.00000000E+00
 V16    -8.85034461E+00   -8.85034461E+00   -8.85034461E+00    0.00000000E+00
 V17     3.16285525E+03    3.16285525E+03    3.16285525E+03    0.00000000E+00
 V19     2.20452445E+04    2.20452445E+04    2.20452445E+04    0.00000000E+00
 V20    -7.16035825E+00   -7.16035825E+00   -7.16035825E+00    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   9.41736381E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   4.28061991E-02


 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0425838E+04
   4 V2        48000000 -2.9544913E+01
  13 V11       48000000 -2.1810205E+04
  14 V12       48000000  1.5161309E+01
  17 V15       48000000  2.4524473E+04
  18 V16       48000000 -8.8503446E+00
  19 V17       48000000  3.1628552E+03
  21 V19       48000000  2.2045244E+04
  22 V20       48000000 -7.1603583E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
```

```
1 T=1193                          1192.      10.0      -1.229     -0.1229
1 W(LIQUID,B)=0.408              0.4084     2.00E-02  3.7523E-04  1.8762E-02
1 W(BCC,B)=0.13                  0.1316     2.00E-02  1.5783E-03  7.8915E-02
2 T=1341                          1342.      10.0      0.6112      6.1120E-02
2 HTR=3727                        3678.      5.00E+02  -48.99     -9.7983E-02
3 T=1049                          1047.      10.0      -1.656     -0.1656
3 W(LIQUID,A)=0.27               0.2711     2.00E-02  1.1419E-03  5.7097E-02
3 W(BCC,A)=9.3E-2                9.5355E-02  2.00E-02  2.3545E-03  0.1177
4 T=1203                          1212.      10.0       8.861      0.8861
4 W(LIQUID,A)=0.19               0.1866     2.00E-02 -3.3513E-03 -0.1676
4 W(BCC,A)=6.9E-2                6.9443E-02  2.00E-02  4.4257E-04  2.2128E-02
4 W(FCC,A)=6E-2                  5.9624E-02  2.00E-02 -3.7607E-04 -1.8803E-02
5 T=726                           724.5      10.0      -1.539     -0.1539
5 X(BCC,B)=3.7E-2                3.6651E-02  2.00E-02 -3.4874E-04 -1.7437E-02
5 X(BCC#2,A)=0.114               0.1147     2.00E-02  7.2219E-04  3.6109E-02
6 X(BCC,B)=3.7E-2                3.7085E-02  2.00E-02  8.4561E-05  4.2281E-03
6 X(BCC#2,A)=0.114               0.1158     2.00E-02  1.8050E-03  9.0250E-02
10 W(LIQUID,A)=2E-2              1.9560E-02  2.00E-02 -4.3955E-04 -2.1977E-02
11 W(LIQUID,A)=4.2E-2            4.1817E-02  2.00E-02 -1.8316E-04 -9.1582E-03
12 W(LIQUID,A)=6.5E-2            6.4841E-02  2.00E-02 -1.5941E-04 -7.9707E-03
13 W(LIQUID,A)=9.3E-2            9.2553E-02  2.00E-02 -4.4677E-04 -2.2338E-02
20 W(LIQUID,A)=0.104             0.1036     2.00E-02 -3.8733E-04 -1.9366E-02
20 W(FCC,A)=3.8E-2               3.8361E-02  2.00E-02  3.6086E-04  1.8043E-02
21 W(LIQUID,A)=0.136             0.1362     2.00E-02  1.9705E-04  9.8524E-03
21 W(FCC,A)=4.7E-2               4.7373E-02  2.00E-02  3.7286E-04  1.8643E-02
22 W(LIQUID,A)=0.187             0.1862     2.00E-02 -7.9389E-04 -3.9695E-02
22 W(FCC,A)=5.9E-2               5.9524E-02  2.00E-02  5.2371E-04  2.6185E-02
23 W(LIQUID,A)=0.245             0.2452     2.00E-02  1.9320E-04  9.6601E-03
23 W(BCC,A)=8.5E-2               8.7003E-02  2.00E-02  2.0035E-03  0.1002


PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    9.41736381E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    9.42553951E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    9.44643142E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    9.18434003E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    9.28574725E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    9.20479911E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    9.35680621E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    9.11696096E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    2.18168252E-01
  1  1.0000E+00   2  9.9999E-01   3  1.0034E+00   4  9.9857E-01   5  9.9971E-01
  6  9.9757E-01   7  1.0011E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    2.07235143E-01
  1  9.9990E-01   2  1.0000E+00   3  1.0024E+00   4  9.9680E-01   5  9.9848E-01
  6  9.9610E-01   7  9.9760E-01

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    1.87994192E-01
  1  9.9973E-01   2  9.9985E-01   3  1.0004E+00   4  9.9280E-01   5  9.9574E-01
  6  9.9339E-01   7  9.9099E-01

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.62151889E-01
  1  9.9932E-01   2  9.9968E-01   3  9.9655E-01   4  9.8495E-01   5  9.9036E-01
  6  9.8792E-01   7  9.7763E-01

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50053570E-01
  1  9.9877E-01   2  9.9938E-01   3  9.9141E-01   4  9.7448E-01   5  9.8315E-01
  6  9.8103E-01   7  9.6066E-01

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   12 iterations
  1  9.9877E-01   2  9.9938E-01   3  9.9141E-01   4  9.7448E-01   5  9.8315E-01
  6  9.8103E-01   7  9.6066E-01

  1 -1.1651E-01   2  1.0617E-02   3  6.2552E-02   4  6.6364E-02   5 -8.1216E-02
  6 -2.1958E-01   7  4.1235E-02   8  8.3058E-02   9  2.9863E-02  10  2.5417E-02
 11  4.5304E-02  12  5.9829E-02  13 -1.7379E-01  14  1.8247E-02  15  4.5330E-02
 16  4.3059E-02  17  1.0640E-01  18 -2.3843E-02  19 -1.1306E-02  20 -8.6872E-03
 21 -1.9428E-02  22 -1.4518E-02  23  2.3484E-02  24  2.1765E-02  25  3.3281E-02
 26 -1.3748E-02  27  6.4932E-02  28 -2.4111E-02  29  5.6807E-02

               THE SUM OF SQUARES IS   1.50053570E-01
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:56



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  13
```

```
 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04006875E+04    2.04258378E+04    2.04258378E+04    2.41616566E-02
 V2     -2.95264884E+01   -2.95449125E+01   -2.95449125E+01    1.31557074E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43137486E+04    2.45244730E+04    2.45244730E+04    7.66766133E-02
 V16    -8.62447823E+00   -8.85034461E+00   -8.85034461E+00    2.08107836E-01
 V17     3.10957097E+03    3.16285525E+03    3.16285525E+03    2.22191980E-01
 V19     2.16271390E+04    2.20452445E+04    2.20452445E+04    4.98933483E-01
 V20    -6.87864884E+00   -7.16035825E+00   -7.16035825E+00    1.22727290E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   9.41736381E-01 TO   1.50053570E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   6.82061684E-03


 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0400688E+04
   4 V2        48000000 -2.9526488E+01
  13 V11       48000000 -2.1810205E+04
  14 V12       48000000  1.5161309E+01
  17 V15       48000000  2.4313749E+04
  18 V16       48000000 -8.6244782E+00
  19 V17       48000000  3.1095710E+03
  21 V19       48000000  2.1627139E+04
  22 V20       48000000 -6.8786488E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.       10.0       -1.165      -0.1165
1 W(LIQUID,B)=0.408              0.4082      2.00E-02  2.1234E-04  1.0617E-02
1 W(BCC,B)=0.13                  0.1313      2.00E-02  1.2510E-03  6.2552E-02
2 T=1341                          1342.       10.0       0.6636      6.6364E-02
2 HTR=3727                        3686.      5.00E+02  -40.61       -8.1216E-02
3 T=1049                          1047.       10.0       -2.196      -0.2196
3 W(LIQUID,A)=0.27               0.2708      2.00E-02  8.2469E-04  4.1235E-02
3 W(BCC,A)=9.3E-2                9.4661E-02  2.00E-02  1.6612E-03  8.3058E-02
4 T=1203                          1203.       10.0       0.2986      2.9863E-02
4 W(LIQUID,A)=0.19               0.1905      2.00E-02  5.0833E-04  2.5417E-02
4 W(BCC,A)=6.9E-2                6.9906E-02  2.00E-02  9.0608E-04  4.5304E-02
4 W(FCC,A)=6E-2                  6.1197E-02  2.00E-02  1.1966E-03  5.9829E-02
5 T=726                           724.3       10.0       -1.738      -0.1738
5 X(BCC,B)=3.7E-2                3.7365E-02  2.00E-02  3.6493E-04  1.8247E-02
5 X(BCC#2,A)=0.114               0.1149      2.00E-02  9.0661E-04  4.5330E-02
6 X(BCC,B)=3.7E-2                3.7861E-02  2.00E-02  8.6118E-04  4.3059E-02
6 X(BCC#2,A)=0.114               0.1161      2.00E-02  2.1279E-03  0.1064
10 W(LIQUID,A)=2E-2              1.9523E-02  2.00E-02 -4.7686E-04 -2.3843E-02
11 W(LIQUID,A)=4.2E-2            4.1774E-02  2.00E-02 -2.2612E-04 -1.1306E-02
12 W(LIQUID,A)=6.5E-2            6.4826E-02  2.00E-02 -1.7374E-04 -8.6872E-03
```

```
13 W(LIQUID,A)=9.3E-2            9.2611E-02  2.00E-02 -3.8856E-04 -1.9428E-02
20 W(LIQUID,A)=0.104             0.1037      2.00E-02 -2.9035E-04 -1.4518E-02
20 W(FCC,A)=3.8E-2               3.8470E-02  2.00E-02  4.6968E-04  2.3484E-02
21 W(LIQUID,A)=0.136             0.1364      2.00E-02  4.3530E-04  2.1765E-02
21 W(FCC,A)=4.7E-2               4.7666E-02  2.00E-02  6.6563E-04  3.3281E-02
22 W(LIQUID,A)=0.187             0.1867      2.00E-02 -2.7497E-04 -1.3748E-02
22 W(FCC,A)=5.9E-2               6.0299E-02  2.00E-02  1.2986E-03  6.4932E-02
23 W(LIQUID,A)=0.245             0.2445      2.00E-02 -4.8222E-04 -2.4111E-02
23 W(BCC,A)=8.5E-2               8.6136E-02  2.00E-02  1.1361E-03  5.6807E-02


PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Now optimize all parameters and all experiments
PARROT: l-a-v
   ... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04006875E+04    2.04258378E+04    2.04258378E+04    2.41616566E-02
 V2     -2.95264884E+01   -2.95449125E+01   -2.95449125E+01    1.31557074E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43137486E+04    2.45244730E+04    2.45244730E+04    7.66766133E-02
 V16    -8.62447823E+00   -8.85034461E+00   -8.85034461E+00    2.08107836E-01
 V17     3.10957097E+03    3.16285525E+03    3.16285525E+03    2.22191980E-01
 V19     2.16271390E+04    2.20452445E+04    2.20452445E+04    4.98933483E-01
 V20    -6.87864884E+00   -7.16035825E+00   -7.16035825E+00    1.22727290E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   9.41736381E-01 TO   1.50053570E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   6.82061684E-03
PARROT: s-o-v 11-12
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
   ... the command in full is READ_WORKSPACES
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1191.8      LIQUID A2B BCC
   2 AINV   2   1.    1341.7      LIQUID A2B
   3 AINV   2   1.    1046.8      LIQUID A2B BCC
   4 AINV   2   1.    1203.3      LIQUID BCC FCC
   5 AINV   2   1.     724.3      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    2   1.    1594.0      LIQUID FCC
  11 ALF    2   1.    1548.0      LIQUID FCC
  12 ALF    2   1.    1499.0      LIQUID FCC
  13 ALF    2   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA   < unused > 1573.0      LIQUID
 101 AA   < unused > 1573.0      LIQUID
 102 AA   < unused > 1573.0      LIQUID
 103 AA   < unused > 1573.0      LIQUID
 104 AA   < unused > 1573.0      LIQUID
 105 AA   < unused > 1573.0      LIQUID
 106 AA   < unused > 1573.0      LIQUID
 107 AA   < unused > 1573.0      LIQUID
 108 AA   < unused > 1573.0      LIQUID
 110 AH   < unused > 1773.0      LIQUID
 111 AH   < unused > 1773.0      LIQUID
 112 AH   < unused > 1773.0      LIQUID
 113 AH   < unused > 1773.0      LIQUID
 114 AH   < unused > 1773.0      LIQUID
 115 AH   < unused > 1773.0      LIQUID
 116 AH   < unused > 1773.0      LIQUID
 117 AH   < unused > 1773.0      LIQUID
 118 AH   < unused > 1773.0      LIQUID
ED_EXP: s-we 1 100-118
   ... the command in full is SET_WEIGHT
ED_EXP: s-e 1
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number                      1 , label AINV
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1191.8      LIQUID A2B BCC
   2 AINV   2   1.    1341.7      LIQUID A2B
   3 AINV   2   1.    1046.8      LIQUID A2B BCC
   4 AINV   2   1.    1203.3      LIQUID BCC FCC
   5 AINV   2   1.     724.3      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    2   1.    1594.0      LIQUID FCC
  11 ALF    2   1.    1548.0      LIQUID FCC
  12 ALF    2   1.    1499.0      LIQUID FCC
  13 ALF    2   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
```

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 115 AH      2   1.    1773.0      LIQUID
 116 AH      2   1.    1773.0      LIQUID
 117 AH      2   1.    1773.0      LIQUID
 118 AH      2   1.    1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    1.71348983E-01
  1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0000E+00   5  9.9141E-01
  6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    1.72203930E-01
  1  9.9887E-01   2  9.9938E-01   3  1.0000E+00   4  1.0000E+00   5  9.9141E-01
  6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    1.74167084E-01
  1  9.9877E-01   2  9.9948E-01   3  1.0000E+00   4  1.0000E+00   5  9.9141E-01
  6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.75634356E-01
  1  9.9877E-01   2  9.9938E-01   3  1.0001E+00   4  1.0000E+00   5  9.9141E-01
  6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69474652E-01
  1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
  6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69562798E-01
  1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9151E-01
  6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69566267E-01
  1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
  6  9.7458E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69484800E-01
  1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
  6  9.7448E-01   7  9.8325E-01   8  9.8103E-01   9  9.6066E-01

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69600694E-01
  1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
  6  9.7448E-01   7  9.8315E-01   8  9.8113E-01   9  9.6066E-01

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69486726E-01
  1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
  6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6076E-01

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    1.52786177E-01
  1  9.9900E-01   2  9.9895E-01   3  9.9938E-01   4  1.0004E+00   5  9.9144E-01
  6  9.7447E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.40532739E-01
  1  9.9890E-01   2  9.9900E-01   3  9.9926E-01   4  1.0005E+00   5  9.9136E-01
  6  9.7393E-01   7  9.8302E-01   8  9.8140E-01   9  9.6114E-01

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.29724490E-01
  1  9.9893E-01   2  9.9866E-01   3  9.9885E-01   4  1.0007E+00   5  9.9142E-01
  6  9.7290E-01   7  9.8276E-01   8  9.8209E-01   9  9.6210E-01

      AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    1.15934436E-01
  1  9.9874E-01   2  9.9848E-01   3  9.9859E-01   4  1.0010E+00   5  9.9102E-01
  6  9.7065E-01   7  9.8221E-01   8  9.8360E-01   9  9.6396E-01

      AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    9.75379513E-02
  1  9.9849E-01   2  9.9788E-01   3  9.9801E-01   4  1.0015E+00   5  9.9032E-01
  6  9.6628E-01   7  9.8112E-01   8  9.8668E-01   9  9.6777E-01

      AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    7.50720931E-02
  1  9.9786E-01   2  9.9702E-01   3  9.9725E-01   4  1.0024E+00   5  9.8867E-01
  6  9.5729E-01   7  9.7889E-01   8  9.9265E-01   9  9.7533E-01

      AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    6.73903735E-02
  1  9.9721E-01   2  9.9606E-01   3  9.9646E-01   4  1.0033E+00   5  9.8691E-01
  6  9.4769E-01   7  9.7652E-01   8  9.9896E-01   9  9.8321E-01

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   16 iterations
  1  9.9721E-01   2  9.9606E-01   3  9.9646E-01   4  1.0033E+00   5  9.8691E-01
  6  9.4769E-01   7  9.7652E-01   8  9.9896E-01   9  9.8321E-01

  1 -5.7769E-02   2 -9.3761E-03   3  1.4158E-02   4  2.0690E-02   5 -2.5688E-02
  6 -5.1171E-02   7  1.9343E-02   8  2.7056E-02   9  1.2439E-02  10  2.7688E-02
 11  9.1632E-03  12  1.3813E-02  13 -4.8791E-02  14  2.1460E-02  15  4.7007E-03
 16  2.8358E-02  17  2.1568E-02  18 -2.2454E-02  19 -8.9460E-03  20 -5.8150E-03
 21 -1.6458E-02  22 -1.1654E-02  23  1.4345E-02  24  2.3824E-02  25  1.4109E-02
 26 -1.4553E-02  27  2.0708E-02  28 -1.2425E-02  29  1.5727E-02  30 -9.5825E-03
 31 -1.6802E-02  32  2.7496E-02  33  8.7112E-02  34  1.2446E-01  35  1.0182E-01
 36 -1.7174E-02  37  7.0704E-02  38 -1.9397E-02  39  1.6052E-02  40  4.5425E-02
 41  4.8120E-02  42  4.6137E-02  43  4.1476E-02  44  3.4137E-02  45  2.2120E-02
 46  7.4249E-03  47 -1.1948E-02

               THE SUM OF SQUARES IS   6.73903735E-02
PARROT: l-r C SCREEN
   ... the command in full is LIST_RESULT


           ===================================================
           OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:56



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  17


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
```

```
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03




 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03688341E+04    2.04258378E+04    2.04258378E+04    2.96135417E-02
 V2     -2.94286301E+01   -2.95449125E+01   -2.95449125E+01    2.25274567E-02
 V11    -2.17330472E+04   -2.18102047E+04   -2.18102047E+04    3.47407502E-02
 V12     1.52107324E+01    1.51613087E+01    1.51613087E+01    5.56505566E-02
 V15     2.42035190E+04    2.45244730E+04    2.45244730E+04    8.09093794E-02
 V16    -8.38741946E+00   -8.85034461E+00   -8.85034461E+00    2.37193886E-01
 V17     3.08858371E+03    3.16285525E+03    3.16285525E+03    2.23457303E-01
 V19     2.20222843E+04    2.20452445E+04    2.20452445E+04    4.94492773E-01
 V20    -7.04010396E+00   -7.16035825E+00   -7.16035825E+00    1.21662443E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.71348983E-01 TO   6.73903735E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.77343088E-03


 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
   3 V1        48000000  2.0368834E+04
   4 V2        48000000 -2.9428630E+01
  13 V11       48000000 -2.1733047E+04
  14 V12       48000000  1.5210732E+01
  17 V15       48000000  2.4203519E+04
  18 V16       48000000 -8.3874195E+00
  19 V17       48000000  3.0885837E+03
  21 V19       48000000  2.2022284E+04
  22 V20       48000000 -7.0401040E+00



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.      10.0     -0.5777     -5.7769E-02
1 W(LIQUID,B)=0.408              0.4078      2.00E-02 -1.8752E-04 -9.3761E-03
1 W(BCC,B)=0.13                  0.1303      2.00E-02  2.8316E-04  1.4158E-02
2 T=1341                          1341.      10.0      0.2069      2.0690E-02
2 HTR=3727                        3714.      5.00E+02  -12.84     -2.5688E-02
3 T=1049                          1048.      10.0     -0.5117     -5.1171E-02
3 W(LIQUID,A)=0.27               0.2704      2.00E-02  3.8687E-04  1.9343E-02
3 W(BCC,A)=9.3E-2                9.3541E-02  2.00E-02  5.4112E-04  2.7056E-02
4 T=1203                          1203.      10.0      0.1244      1.2439E-02
4 W(LIQUID,A)=0.19               0.1906      2.00E-02  5.5376E-04  2.7688E-02
4 W(BCC,A)=6.9E-2                6.9183E-02  2.00E-02  1.8326E-04  9.1632E-03
4 W(FCC,A)=6E-2                  6.0276E-02  2.00E-02  2.7626E-04  1.3813E-02
5 T=726                           725.5      10.0     -0.4879     -4.8791E-02
5 X(BCC,B)=3.7E-2                3.7429E-02  2.00E-02  4.2920E-04  2.1460E-02
5 X(BCC#2,A)=0.114               0.1141      2.00E-02  9.4014E-05  4.7007E-03
6 X(BCC,B)=3.7E-2                3.7567E-02  2.00E-02  5.6715E-04  2.8358E-02
6 X(BCC#2,A)=0.114               0.1144      2.00E-02  4.3136E-04  2.1568E-02
10 W(LIQUID,A)=2E-2              1.9551E-02  2.00E-02 -4.4908E-04 -2.2454E-02
11 W(LIQUID,A)=4.2E-2            4.1821E-02  2.00E-02 -1.7892E-04 -8.9460E-03
12 W(LIQUID,A)=6.5E-2            6.4884E-02  2.00E-02 -1.1630E-04 -5.8150E-03
13 W(LIQUID,A)=9.3E-2            9.2671E-02  2.00E-02 -3.2917E-04 -1.6458E-02
20 W(LIQUID,A)=0.104             0.1038      2.00E-02 -2.3309E-04 -1.1654E-02
20 W(FCC,A)=3.8E-2               3.8287E-02  2.00E-02  2.8690E-04  1.4345E-02
21 W(LIQUID,A)=0.136             0.1365      2.00E-02  4.7648E-04  2.3824E-02
21 W(FCC,A)=4.7E-2               4.7282E-02  2.00E-02  2.8217E-04  1.4109E-02
```

```
22 W(LIQUID,A)=0.187             0.1867      2.00E-02 -2.9105E-04 -1.4553E-02
22 W(FCC,A)=5.9E-2               5.9414E-02  2.00E-02  4.1416E-04  2.0708E-02
23 W(LIQUID,A)=0.245             0.2448      2.00E-02 -2.4851E-04 -1.2425E-02
23 W(BCC,A)=8.5E-2               8.5315E-02  2.00E-02  3.1454E-04  1.5727E-02
100 ACR(B)=0.94                  0.9397      2.85E-02 -2.7275E-04 -9.5825E-03
101 ACR(B)=0.84                  0.8395      2.82E-02 -4.7358E-04 -1.6802E-02
102 ACR(B)=0.74                  0.7408      2.81E-02  7.7139E-04  2.7496E-02
103 ACR(B)=0.64                  0.6424      2.81E-02  2.4449E-03  8.7112E-02
104 ACR(B)=0.54                  0.5435      2.82E-02  3.5129E-03  0.1245
105 ACR(B)=0.44                  0.4429      2.85E-02  2.9062E-03  0.1018
106 ACR(B)=0.34                  0.3395      2.90E-02 -4.9853E-04 -1.7174E-02
107 ACR(B)=0.23                  0.2321      2.97E-02  2.1003E-03  7.0704E-02
108 ACR(B)=0.12                  0.1194      3.06E-02 -5.9355E-04 -1.9397E-02
110 HMR(LIQUID)=-1964            -1956.      5.00E+02   8.026      1.6052E-02
111 HMR(LIQUID)=-3500            -3477.      5.00E+02   22.71      4.5425E-02
112 HMR(LIQUID)=-4588            -4564.      5.00E+02   24.06      4.8120E-02
113 HMR(LIQUID)=-5239            -5216.      5.00E+02   23.07      4.6137E-02
114 HMR(LIQUID)=-5454            -5433.      5.00E+02   20.74      4.1476E-02
115 HMR(LIQUID)=-5233            -5216.      5.00E+02   17.07      3.4137E-02
116 HMR(LIQUID)=-4575            -4564.      5.00E+02   11.06      2.2120E-02
117 HMR(LIQUID)=-3481            -3477.      5.00E+02   3.712      7.4249E-03
118 HMR(LIQUID)=-1950            -1956.      5.00E+02  -5.974     -1.1948E-02


PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram a final time.
PARROT: mac tcex36cpd
   ... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
```

```
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28

Phase region boundary   1 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at axis limit.

Phase region boundary   2 at:   7.141E-01  3.000E+02
    BCC
 ** BCC#2
Calculated.                     14  equilibria

Phase region boundary   3 at:   6.819E-01  7.255E+02
 ** A2B
    BCC
 ** BCC#2

Phase region boundary   4 at:   3.626E-01  7.255E+02
 ** A2B
    BCC
Calculated.                     15  equilibria

Phase region boundary   5 at:   3.771E-01  1.192E+03
 ** LIQUID
 ** A2B
    BCC

Phase region boundary   6 at:   2.828E-01  1.192E+03
 ** LIQUID
    BCC
Calculated                     29  equilibria

Phase region boundary   7 at:   4.863E-01  1.192E+03
 ** LIQUID
    A2B
Calculated.                     28  equilibria

Phase region boundary   8 at:   6.500E-01  1.048E+03
 ** LIQUID
    A2B
 ** BCC

Phase region boundary   9 at:   7.639E-01  1.048E+03
    A2B
 ** BCC
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.272E-01  1.048E+03
    LIQUID
 ** BCC
Calculated.                      8  equilibria

Phase region boundary  11 at:   8.748E-01  1.203E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.799E-01  1.203E+03
    LIQUID
 ** FCC
Calculated                     33  equilibria

Phase region boundary  13 at:   9.353E-01  1.203E+03
    BCC
 ** FCC
Calculated                     22  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.
```

```
Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                      2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.647E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  26 at:   3.647E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.647E-01  7.700E+02
 ** A2B
    BCC
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.910E-01  7.700E+02
 ** A2B
    BCC
Calculated                     10  equilibria

Phase region boundary  29 at:   7.910E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.910E-01  7.700E+02
 ** A2B
    BCC
Calculated.                      9  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.448E-01  1.230E+03
 ** LIQUID
    BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.448E-01  1.230E+03
 ** LIQUID
    BCC
Calculated                     26  equilibria

Phase region boundary  33 at:   8.858E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.858E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                     29  equilibria

Phase region boundary  35 at:   6.415E-03  1.397E+03
    LIQUID
 ** BCC
Calculated                     13  equilibria

Phase region boundary  36 at:   6.415E-03  1.397E+03
    LIQUID
 ** BCC
Calculated.                     13  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.299E-01  1.244E+03
    LIQUID
 ** BCC
Calculated                     20  equilibria

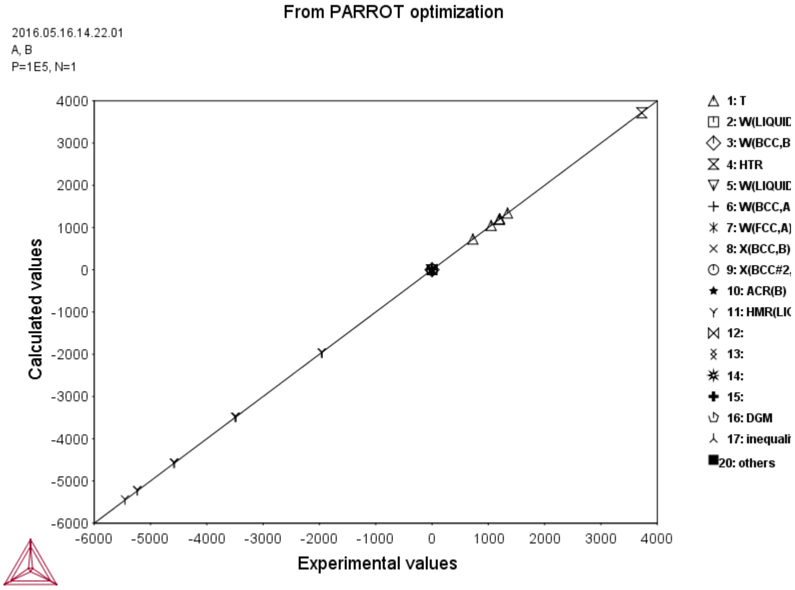
Phase region boundary  38 at:   2.299E-01  1.244E+03
    LIQUID
 ** BCC
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.240E+03
    LIQUID
 ** A2B
Calculated.                     14  equilibria
Terminating at known equilibrium
```

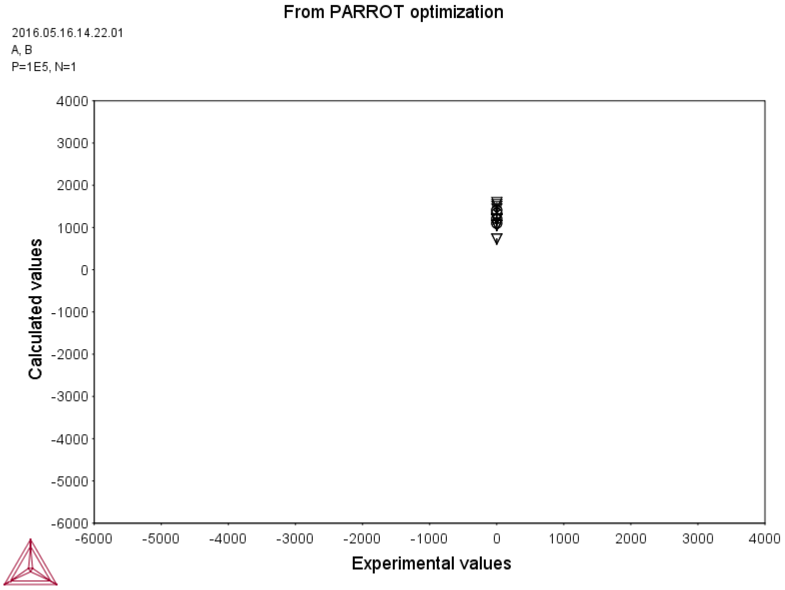
```
 Phase region boundary  40 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated.                       8  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                      20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      13  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                      1  seconds
POLY_3: post
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ Add the experimental data
POST: a-e-d y exp36 0; 1
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
   ... the command in full is BACK
POLY_3: read,,,
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-c t=1773
   ... the command in full is SET_CONDITION
```

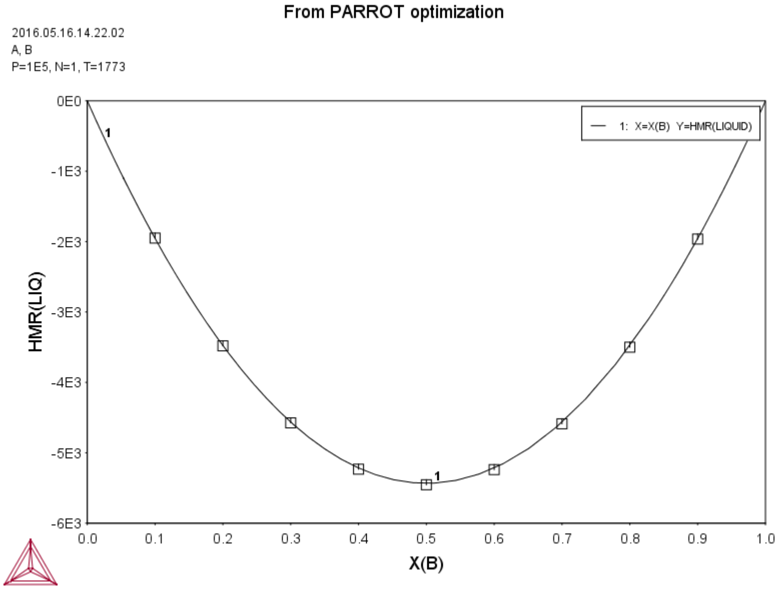
```
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
POLY_3: sh hmr
   ... the command in full is SHOW_VALUE
 HMR=13116.464
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 A                        ENTERED   SER
 B                        ENTERED   SER
POLY_3: s-r-s a liq * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s b liq * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: save tcex36h y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.123400
...OK

 Phase Region from   0.123400     for:
     LIQUID
 Global test at  3.23400E-01 .... OK
 Global test at  5.73400E-01 .... OK
 Global test at  8.23400E-01 .... OK
 Global test at  9.53400E-01 .... OK
 Global test at  1.00000E+00 .... OK
 Terminating at    1.00000
 Calculated    51 equilibria

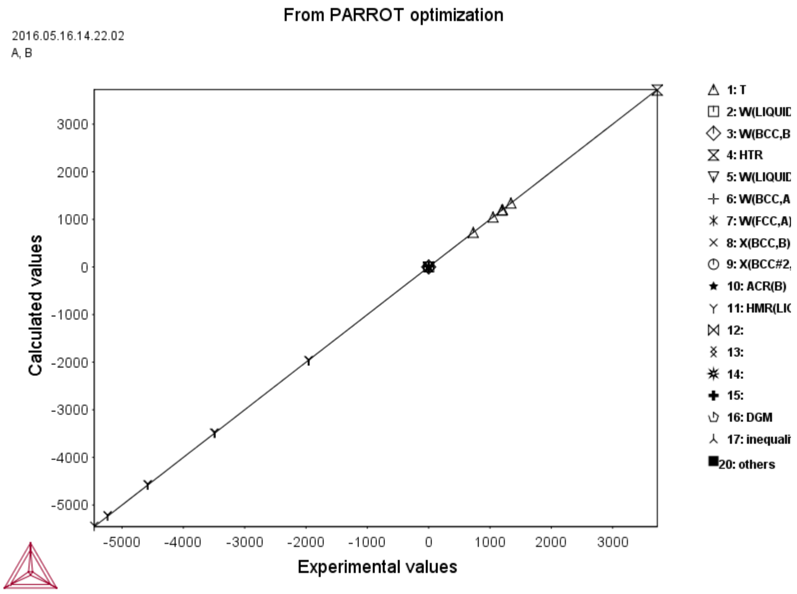
 Phase Region from   0.123400     for:
     LIQUID
 Global test at  8.34000E-02 .... OK
 Global test at  3.34000E-02 .... OK
 Terminating at   0.250000E-11
 Calculated    28 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36h.POLY3
POLY_3: post
POST: s-d-a x x(b)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y hmr(liq)
   ... the command in full is SET_DIAGRAM_AXIS
POST: a-e-d y exp36 0; 2
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



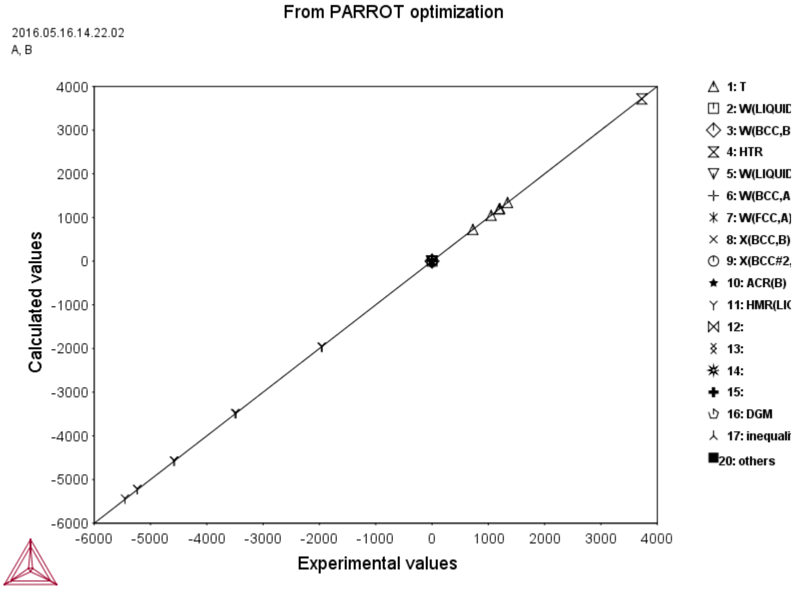
```
POST:
POST:Hit RETURN to continue
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-result gra pexp36 1,
   ... the command in full is LIST_RESULT
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is PLOT_DIAGRAM
```



```
POST: s-s-s y n -6000 4000
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s x n -6000 4000
   ... the command in full is SET_SCALING_STATUS
POST: pl
   ... the command in full is PLOT_DIAGRAM
```



```
POST: b
   ... the command in full is BACK
PARROT: set-inter
   ... the command in full is SET_INTERACTIVE
PARROT:
```

tcex36a-tcex36cpd

```
PARROT:AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tcex36cpd.TCM" set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC
  ** BCC#2
 Calculated..                         2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC
  ** BCC#2
 Calculated.                        14  equilibria

 Phase region boundary   3 at:   6.819E-01  7.255E+02
  ** A2B
     BCC
  ** BCC#2

 Phase region boundary   4 at:   3.626E-01  7.255E+02
```

```
 ** A2B
    BCC
Calculated.                      15  equilibria

Phase region boundary   5 at:   3.771E-01  1.192E+03
 ** LIQUID
 ** A2B
    BCC

Phase region boundary   6 at:   2.828E-01  1.192E+03
 ** LIQUID
    BCC
Calculated                      29  equilibria

Phase region boundary   7 at:   4.863E-01  1.192E+03
 ** LIQUID
    A2B
Calculated.                      28  equilibria

Phase region boundary   8 at:   6.500E-01  1.048E+03
 ** LIQUID
    A2B
 ** BCC

Phase region boundary   9 at:   7.639E-01  1.048E+03
    A2B
 ** BCC
Calculated.                      11  equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.272E-01  1.048E+03
    LIQUID
 ** BCC
Calculated.                       8  equilibria

Phase region boundary  11 at:   8.748E-01  1.203E+03
    LIQUID
 ** BCC
 ** FCC

Phase region boundary  12 at:   8.799E-01  1.203E+03
    LIQUID
 ** FCC
Calculated                      33  equilibria

Phase region boundary  13 at:   9.353E-01  1.203E+03
    BCC
 ** FCC
Calculated                      22  equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC
 ** BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated.                      13  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC
    BCC#2
Calculated..                       2  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
```

```
  ** BCC
     BCC#2
 Calculated.                     13  equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   3.647E-01  7.700E+02
  ** A2B
     BCC
 Calculated                     10  equilibria

 Phase region boundary  26 at:   3.647E-01  7.700E+02
  ** A2B
     BCC
 Calculated.                      3  equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   3.647E-01  7.700E+02
  ** A2B
     BCC
 Calculated.                     14  equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.910E-01  7.700E+02
  ** A2B
     BCC
 Calculated                     10  equilibria

 Phase region boundary  29 at:   7.910E-01  7.700E+02
  ** A2B
     BCC
 Calculated.                      3  equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.910E-01  7.700E+02
  ** A2B
     BCC
 Calculated.                      9  equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.448E-01  1.230E+03
  ** LIQUID
     BCC
 Calculated.                      4  equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.448E-01  1.230E+03
  ** LIQUID
     BCC
 Calculated                     26  equilibria

 Phase region boundary  33 at:   8.858E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                      2  equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.858E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                     29  equilibria

 Phase region boundary  35 at:   6.415E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated                     13  equilibria

 Phase region boundary  36 at:   6.415E-03  1.397E+03
     LIQUID
  ** BCC
 Calculated.                     13  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC
 Calculated                     20  equilibria

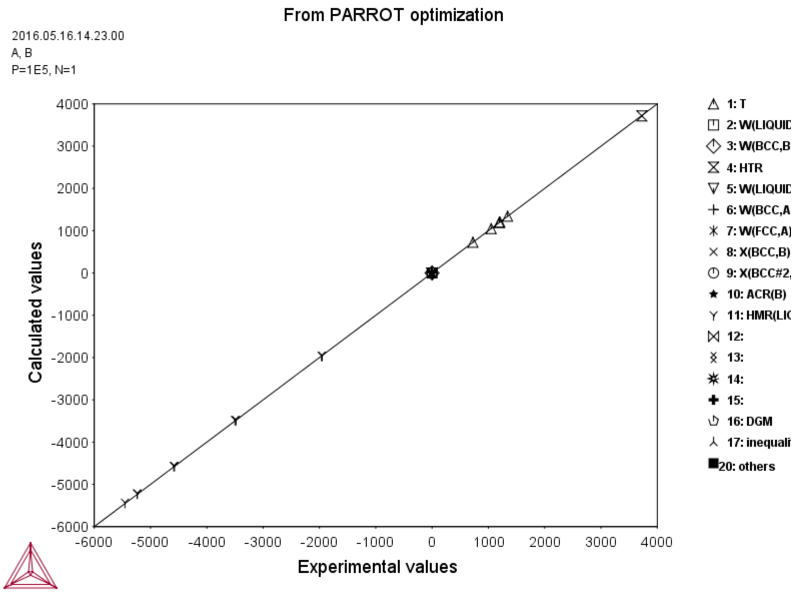
 Phase region boundary  38 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC
 Calculated.                      4  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated.                     14  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated.                      8  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                     20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                     13  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
 x36.POLY3
 CPU time for mapping                     1  seconds
POLY_3: post
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex37

```
About Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex37\tcex37.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of an isothermal section, using command-lines
SYS: @@
SYS: set-log tcex37,,
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw fedemo
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys
   ... the command in full is DEFINE_SYSTEM
ELEMENTS: fe cr ni
 FE                      CR                      NI
   DEFINED
TDB_FEDEMO: l-s c
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :CR FE NI:
 BCC_A2      :CR FE NI:VA:
 CHI_A12     :CR FE NI:CR:CR FE NI:
 FCC_A1      :CR FE NI:VA:
 HCP_A3      :CR FE NI:VA:
 LAVES_PHASE_C14 :CR FE NI:CR FE NI:
 SIGMA       :CR FE NI:CR:CR FE NI:
TDB_FEDEMO:Hit RETURN to continue
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, pp. 1155-1170'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
      (1986); CR-FE-MO'
  'B.-J. Lee, estimated parameter 1999'
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Fe-Cr-Ni'
 -OK-
TDB_FEDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: cps
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 NI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 SIGMA                   ENTERED      0.000000E+00    0.000000E+00
 LAVES_PHASE_C14         ENTERED      0.000000E+00    0.000000E+00
 HCP_A3                  ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                  ENTERED      0.000000E+00    0.000000E+00
 CHI_A12                 ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                  ENTERED      0.000000E+00    0.000000E+00
 LIQUID                  ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CR ENTERED    FE ENTERED    NI ENTERED    VA ENTERED
POLY_3: @@ Set conditions for a point inside the diagram
POLY_3: s-c x(cr)=0.2 x(ni)=0.4
   ... the command in full is SET_CONDITION
POLY_3: s-c t=1673 p=1e5 n=1
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
```

```
 X(CR)=0.2, X(NI)=0.4, T=1673, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         12633 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: FEDEMO

 Conditions:
 X(CR)=0.2, X(NI)=0.4, T=1673, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1673.00 K (  1399.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.62140E+01
 Total Gibbs energy -1.08423E+05,  Enthalpy  4.89973E+04,  Volume  7.34279E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      2.0000E-01  1.8499E-01 7.8623E-04 -9.9434E+04 SER
 FE                      4.0000E-01  3.9739E-01 4.0953E-04 -1.0851E+05 SER
 NI                      4.0000E-01  4.1762E-01 3.0004E-04 -1.1283E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.6214E+01, Volume fraction 1.0000E+00  Mass fractions:
 NI  4.17618E-01  FE  3.97389E-01  CR  1.84993E-01
POLY_3: s-a-v
   ... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: s-a-v 2
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: x(cr)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: save tcex37 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16

 Phase region boundary   1 at:   9.201E-03  4.019E-02
  ** BCC_A2
     FCC_A1
 Calculated                     14  equilibria

 Phase region boundary   2 at:   9.201E-03  4.019E-02
  ** BCC_A2
     FCC_A1
 Calculated.                     31  equilibria

 Phase region boundary   3 at:   1.950E-01  3.373E-01
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary   4 at:   2.267E-01  3.103E-01
  ** LIQUID
     FCC_A1
 Calculated                     53  equilibria

 Phase region boundary   5 at:   1.883E-01  3.539E-01
  ** LIQUID
     BCC_A2
 Calculated                     49  equilibria

 Phase region boundary   6 at:   1.950E-01  3.373E-01
  ** BCC_A2
     FCC_A1
 Calculated                     51  equilibria

 Phase region boundary   7 at:   3.334E-01  3.082E-01
  ** LIQUID
     FCC_A1
 Calculated.                     10  equilibria
```

```
 Terminating at known equilibrium

 Phase region boundary   8 at:   3.334E-01  3.082E-01
  ** LIQUID
     FCC_A1
 Calculated                     39  equilibria

 Phase region boundary   9 at:   6.543E-01  3.046E-01
  ** LIQUID
     FCC_A1
 Calculated.                     35  equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   6.543E-01  3.046E-01
  ** LIQUID
     FCC_A1
 Calculated                     23  equilibria

 Phase region boundary  11 at:   1.678E-01  3.000E-01
     BCC_A2
  ** FCC_A1
 Calculated                     34  equilibria

 Phase region boundary  12 at:   1.678E-01  3.000E-01
     BCC_A2
  ** FCC_A1
 Calculated.                      4  equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   3.086E-01  5.984E-01
  ** LIQUID
     BCC_A2
 Calculated.                     21  equilibria
 Terminating at known equilibrium

 Phase region boundary  14 at:   3.086E-01  5.984E-01
  ** LIQUID
     BCC_A2
 Calculated                     25  equilibria

 Phase region boundary  15 at:   1.097E-02  4.525E-02
     BCC_A2
  ** FCC_A1
 Calculated                     15  equilibria

 Phase region boundary  16 at:   1.097E-02  4.525E-02
     BCC_A2
  ** FCC_A1
 Calculated.                     31  equilibria
 Terminating at known equilibrium

 Phase region boundary  17 at:   3.342E-01  6.558E-01
     LIQUID
  ** BCC_A2
 Calculated.                     26  equilibria
 Terminating at known equilibrium

 Phase region boundary  18 at:   3.342E-01  6.558E-01
     LIQUID
  ** BCC_A2
 Calculated                     13  equilibria

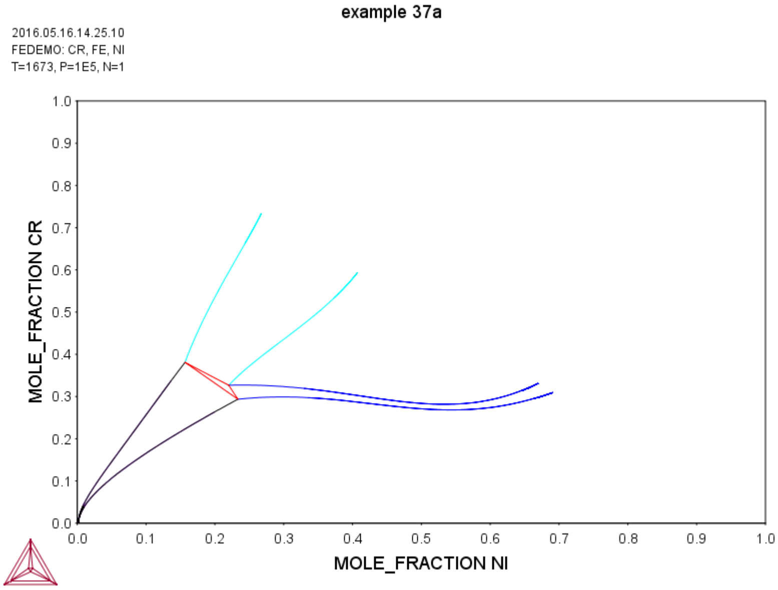
 Phase region boundary  19 at:   6.736E-01  3.160E-01
     LIQUID
  ** FCC_A1
 Calculated.                     37  equilibria
 Terminating at known equilibrium

 Phase region boundary  20 at:   6.736E-01  3.160E-01
     LIQUID
  ** FCC_A1
 Calculated                     18  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex37\tcex
 37.POLY3
 CPU time for mapping                      3  seconds
POLY_3: post

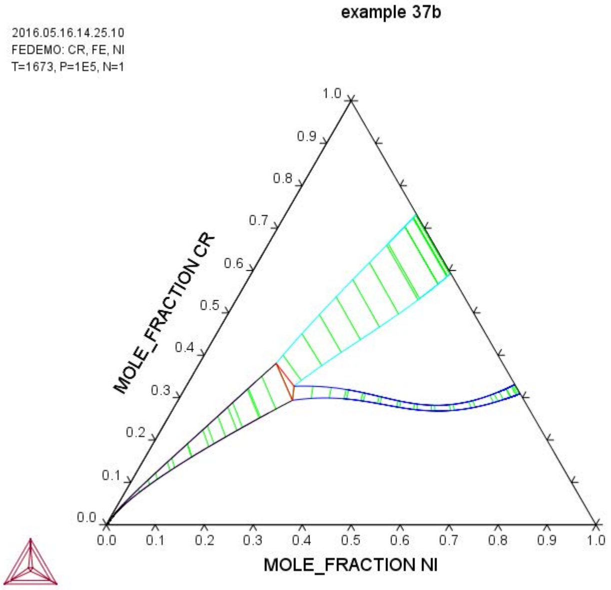
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

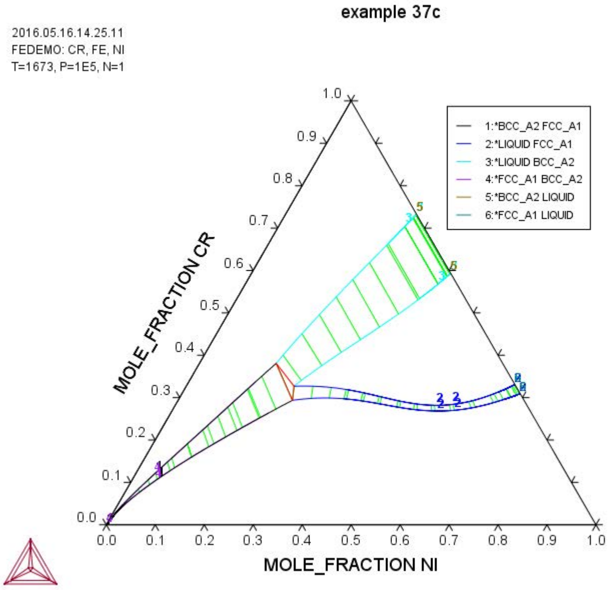
POST: @@ Use default axis on the diagram
POST:
POST: set-title example 37a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ By default a diagram is always square. set it triangular,
POST: @@ add tie-lines and set scaling on the axis
POST: s-d-t
   ... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM  (Y OR N) /N/: y
POST: s-t-s
   ... the command in full is SET_TIELINE_STATUS
PLOTTING EVERY TIE-LINE NO /0/: 3
POST: s-sc
   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING  (Y OR N) /N/: n
MIN VALUE : 0
MAX VALUE : 1
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 37b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ To identify the phases also set labels
POST: @@ To add text in phase regions use a dataplot file
POST: set-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 37c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex38

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex38\tcex38.TCM" set-echo
SYS: @@
SYS: @@ Calculation of the Morral "rose"
SYS: @@
SYS: @@ Calculation of miscibility gaps ...
SYS: @@
SYS: set-log ex38,,,,
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: rei,,,,,,
   ... the command in full is REINITIATE
GES:
GES: @@ Enter a phase with just a ternary interaction parameter
GES: e-e a b c
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
GES: a-e-d a fcc_a1 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d b fcc_a1 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d c fcc_a1 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES:
GES:
GES: e-ph fcc_a1,,1 A B C;,,,,,
   ... the command in full is ENTER_PHASE
GES:
GES:
GES: e-par l(fcc_a1,a,b,c),,50000;,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B,C;0)
GES: l-d
   ... the command in full is LIST_DATA
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE: User data 2016.05.16

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  1 A    FCC_A1                    1.0000E+01  0.0000E+00  0.0000E+00
  2 B    FCC_A1                    1.0000E+01  1.2220E+03  5.9000E+00
  3 C    FCC_A1                    1.0000E+01  1.0540E+03  5.7400E+00


 SPECIES                                    STOICHIOMETRY
   1 A                                      A
   2 B                                      B
   3 C                                      C



 FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B,C

      G(FCC_A1,A;0)-G(FCC_A1,A;0) = 0.0
      G(FCC_A1,B;0)-G(FCC_A1,B;0) = 0.0
      G(FCC_A1,C;0)-G(FCC_A1,C;0) = 0.0
      L(FCC_A1,A,B,C;0) = +50000

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3:
POLY_3: s-c t=600 p=1e5 n=1 x(b)=.3 x(c)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Creating a new composition set FCC_A1#2
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=600, P=1E5, N=1, X(B)=0.3, X(C)=0.1
 DEGREES OF FREEDOM 0

 Temperature    600.00 K (   326.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.58989E+03,  Enthalpy  6.74567E+02,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 5.7356E-01 -2.7732E+03 SER
 B                       3.0000E-01  3.0000E-01 3.8092E-01 -4.8149E+03 SER
 C                       1.0000E-01  1.0000E-01 3.8092E-01 -4.8149E+03 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 8.7781E-01, Mass 8.7781E+00, Volume fraction 0.0000E+00  Mass fractions:
```

```
 A  6.00000E-01  B  3.32342E-01  C  6.76579E-02

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.2219E-01, Mass 1.2219E+00, Volume fraction 0.0000E+00  Mass fractions:
 A  6.00000E-01  C  3.32342E-01  B  6.76579E-02
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 x(b) 0 1 0.01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(c) 0 1 0.01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: save tcex38 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Trying global minimization! 3
 Generating start point   1
 Generating start point   2
 Trying global minimization! 3
 Generating start point   3
 Generating start point   4
 Trying global minimization! 3
 Generating start point   5
 Generating start point   6
 Trying global minimization! 3
 Generating start point   7
 Generating start point   8
 Trying global minimization! 3
 Generating start point   9
 Generating start point  10
 Working hard
 Trying global minimization! 3
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14

 Phase region boundary   1 at:   9.900E-01  1.000E-02
     FCC_A1
  ** FCC_A1#2

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 Phase region boundary   2 at:   9.900E-01  1.000E-02
     FCC_A1
  ** FCC_A1#2

                                                      +                                                    ++

 Phase region boundary   3 at:   2.333E-01  2.333E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                     32  equilibria

 Phase region boundary   4 at:   2.333E-01  2.333E-01
     FCC_A1
  ** FCC_A1#2
 Creating a new composition set FCC_A1#3
 Calculated                     11  equilibria

 Phase region boundary   5 at:   2.333E-01  2.333E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                      5  equilibria

 Phase region boundary   6 at:   2.699E-01  2.699E-01
     FCC_A1
  ** FCC_A1#2
  ** FCC_A1#3

 Phase region boundary   7 at:   4.603E-01  2.699E-01
     FCC_A1
  ** FCC_A1#3
 Calculated                     45  equilibria

 Phase region boundary   8 at:   2.699E-01  4.603E-01
     FCC_A1#2
  ** FCC_A1#3
 Calculated                     55  equilibria

 Phase region boundary   9 at:   2.699E-01  2.699E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                     32  equilibria

 Phase region boundary  10 at:   6.633E-01  1.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                     25  equilibria

 Phase region boundary  11 at:   6.633E-01  1.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                     33  equilibria

 Phase region boundary  12 at:   6.633E-01  1.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                     22  equilibria
 Terminating at known equilibrium
```

```
 Phase region boundary  13 at:   2.333E-01  2.333E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      35  equilibria

 Phase region boundary  14 at:   2.333E-01  2.333E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      11  equilibria

 Phase region boundary  15 at:   2.333E-01  2.333E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                       5  equilibria
 Terminating at known equilibrium

 Phase region boundary  16 at:   1.683E-01  6.633E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      33  equilibria

 Phase region boundary  17 at:   1.683E-01  6.633E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                      22  equilibria
 Terminating at known equilibrium

 Phase region boundary  18 at:   1.683E-01  6.633E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      28  equilibria

 Phase region boundary  19 at:   2.333E-01  5.333E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      20  equilibria

 Phase region boundary  20 at:   2.333E-01  5.333E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                       9  equilibria
 Terminating at known equilibrium

 Phase region boundary  21 at:   2.333E-01  5.333E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      44  equilibria

 Phase region boundary  22 at:   6.633E-01  1.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      25  equilibria

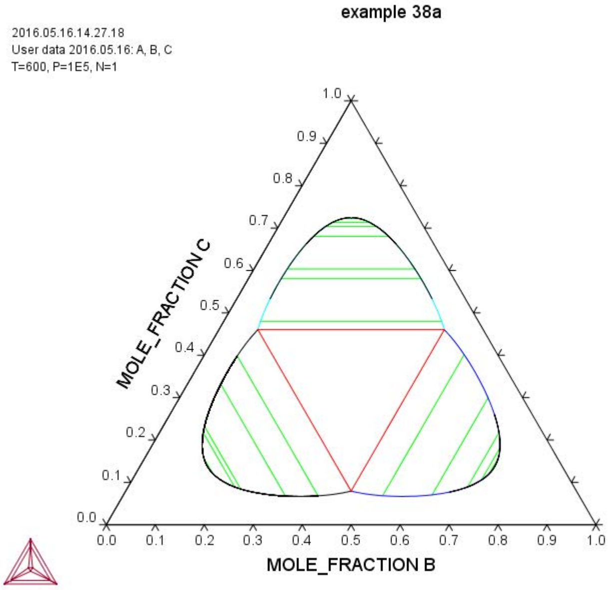
 Phase region boundary  23 at:   6.633E-01  1.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      33  equilibria

 Phase region boundary  24 at:   6.633E-01  1.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                      22  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex38\tcex
 38.POLY3
 CPU time for mapping                      2  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST: s-d-a x m-f b
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y m-f c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-t-s 10
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 38a
POST: plot
   ... the command in full is PLOT_DIAGRAM
 The composition set FCC_A1#3 created from the store file
```



```
POST:
POST:Hit RETURN to continue
POST: back
POLY_3: read,,
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: @@ We will calculate at a higher temperature
POLY_3: @@ with a stable phase in the middle.
POLY_3: s-c t=696
   ... the command in full is SET_CONDITION
POLY_3: s-c x(b)=.44 x(c)=.28
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Creating a new composition set FCC_A1#3
 Calculated POLY solution       0 s, total time     0   s
POLY_3:
POLY_3: save tcex38b y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Working hard
 Trying global minimization! 3
 Generating start point   1
 Generating start point   2
 Trying global minimization! 3
 Generating start point   3
 Generating start point   4
 Trying global minimization! 3
 Generating start point   5
 Generating start point   6

 Phase region boundary   1 at:   2.683E-01  2.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                     33  equilibria

 Phase region boundary   2 at:   2.683E-01  2.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      6  equilibria

 Phase region boundary   3 at:   2.683E-01  2.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      6  equilibria

 Phase region boundary   4 at:   2.683E-01  2.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      6  equilibria

 Phase region boundary   5 at:   2.683E-01  2.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      6  equilibria

 Phase region boundary   6 at:   2.683E-01  2.683E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      6  equilibria

 Phase region boundary   7 at:   2.683E-01  2.683E-01
```

```
    FCC_A1
 ** FCC_A1#2
Calculated.                       6  equilibria

Phase region boundary   8 at:   2.998E-01  2.998E-01
    FCC_A1
 ** FCC_A1#2
 ** FCC_A1#3

Phase region boundary   9 at:   3.618E-01  2.650E-01
    FCC_A1
 ** FCC_A1#3
Calculated                       8  equilibria

Phase region boundary  10 at:   3.618E-01  2.650E-01
    FCC_A1
 ** FCC_A1#3
Calculated.                       6  equilibria

Phase region boundary  11 at:   3.732E-01  2.650E-01
    FCC_A1
 ** FCC_A1#2
 ** FCC_A1#3

Phase region boundary  12 at:   4.004E-01  2.998E-01
    FCC_A1
 ** FCC_A1#2
Calculated                      34  equilibria

Phase region boundary  13 at:   3.732E-01  3.618E-01
 ** FCC_A1#2
    FCC_A1#3
Calculated                       4  equilibria

Phase region boundary  14 at:   3.732E-01  3.618E-01
 ** FCC_A1#2
    FCC_A1#3
Calculated.                       3  equilibria

Phase region boundary  15 at:   3.618E-01  3.732E-01
 ** FCC_A1
 ** FCC_A1#2
    FCC_A1#3

Phase region boundary  16 at:   2.650E-01  3.732E-01
 ** FCC_A1
    FCC_A1#3
Calculated                       9  equilibria

Phase region boundary  17 at:   2.650E-01  3.732E-01
 ** FCC_A1
    FCC_A1#3
Calculated.                       7  equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   2.998E-01  4.004E-01
 ** FCC_A1
    FCC_A1#2
Calculated                      37  equilibria

Phase region boundary  19 at:   2.998E-01  2.998E-01
    FCC_A1
 ** FCC_A1#2
Calculated                      40  equilibria

Phase region boundary  20 at:   2.683E-01  2.683E-01
    FCC_A1
 ** FCC_A1#2
Calculated                      35  equilibria

Phase region boundary  21 at:   2.683E-01  2.683E-01
    FCC_A1
 ** FCC_A1#2
Calculated                       6  equilibria

Phase region boundary  22 at:   2.683E-01  2.683E-01
    FCC_A1
 ** FCC_A1#2
Calculated                       6  equilibria

Phase region boundary  23 at:   2.683E-01  2.683E-01
    FCC_A1
 ** FCC_A1#2
Calculated                       6  equilibria

Phase region boundary  24 at:   2.683E-01  2.683E-01
    FCC_A1
 ** FCC_A1#2
Calculated                       6  equilibria

Phase region boundary  25 at:   2.683E-01  2.683E-01
    FCC_A1
 ** FCC_A1#2
Calculated                       6  equilibria

Phase region boundary  26 at:   2.683E-01  2.683E-01
    FCC_A1
 ** FCC_A1#2
Calculated.                       6  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   2.683E-01  4.633E-01
    FCC_A1
 ** FCC_A1#2
Calculated.                       9  equilibria
Creating a new composition set FCC_A1#4
Calculated                       9  equilibria

Phase region boundary  28 at:   2.683E-01  4.633E-01
    FCC_A1
 ** FCC_A1#2
Calculated                       9  equilibria

Phase region boundary  29 at:   2.683E-01  4.633E-01
    FCC_A1
 ** FCC_A1#2
```

```
 Calculated                         9  equilibria

 Phase region boundary  30 at:   2.683E-01  4.633E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                         9  equilibria

 Phase region boundary  31 at:   2.683E-01  4.633E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                         9  equilibria

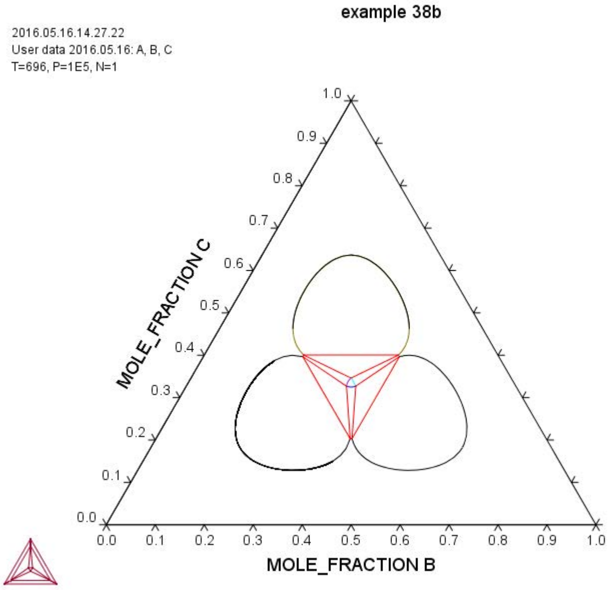
 Phase region boundary  32 at:   2.683E-01  4.633E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                         9  equilibria
 Terminating at known equilibrium

 Phase region boundary  33 at:   2.683E-01  4.633E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                       31  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex38\tcex
 38b.POLY3
 CPU time for mapping                        3  seconds
POLY_3:
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: set-title example 38b
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
 The composition set FCC_A1#4 created from the store file
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: back
POLY_3: @@ ============================================
POLY_3: @@ Now a quaternary!
POLY_3: @@
POLY_3: @@ Square rose by John Morral
POLY_3: @@
POLY_3: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: rei,,,,,
   ... the command in full is REINITIATE
GES: e-e a b c d
   ... the command in full is ENTER_ELEMENT
GES: a-e-d a liquid 10,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d b liquid 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d c liquid 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d d liquid 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: e-ph liquid
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B C D
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES: e-par g(liquid,a,b,c,d)
```

```
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A,B,C,D;0)
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: 100000
&
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: N
GES:
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: rei,,,,
   ... the command in full is REINITIATE_MODULE
POLY_3: s-c t=170 p=1e5 n=1 x(d)=.25 x(a)=.3 x(a)+x(c)=.5
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=170, P=1E5, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          1819 grid points in              0 s
 Creating a new composition set LIQUID#2
    32 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VXCS
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=170, P=1E5, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
 DEGREES OF FREEDOM 0

 Temperature    170.00 K (  -103.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -1.58399E+03,  Enthalpy  2.18612E+02,  Volume  0.00000E+00

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 A                        3.0000E-01  3.0000E-01 3.1587E-01 -1.6289E+03 SER
 B                        2.5000E-01  2.5000E-01 3.5423E-01 -1.4669E+03 SER
 C                        2.0000E-01  2.0000E-01 3.5423E-01 -1.4669E+03 SER
 D                        2.5000E-01  2.5000E-01 2.9182E-01 -1.7409E+03 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.8530E-01, Mass 5.8530E+00, Volume fraction 0.0000E+00  Mole fractions:
 B  3.71549E-01  A  3.00000E-01  D  2.50000E-01  C  7.84507E-02

 LIQUID#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 4.1470E-01, Mass 4.1470E+00, Volume fraction 0.0000E+00  Mole fractions:
 C  3.71549E-01  A  3.00000E-01  D  2.50000E-01  B  7.84507E-02
POLY_3: s-a-v 1 x(a)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .01
POLY_3: s-a-v 2 x(d)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .01
POLY_3:
POLY_3: add +1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: save tcex38c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.478E-01  2.500E-01
     LIQUID
  ** LIQUID#2
 Creating a new composition set LIQUID#3
 Calculated                     6  equilibria

 Phase region boundary   2 at:   4.478E-01  2.500E-01
     LIQUID
  ** LIQUID#2
 Calculated                     2  equilibria

 Phase region boundary   3 at:   4.478E-01  2.500E-01
     LIQUID
  ** LIQUID#2
 Calculated                     2  equilibria

 Phase region boundary   4 at:   4.478E-01  2.500E-01
     LIQUID
  ** LIQUID#2
 Calculated                     2  equilibria

 Phase region boundary   5 at:   4.478E-01  2.500E-01
     LIQUID
  ** LIQUID#2
 Calculated                     2  equilibria

 Phase region boundary   6 at:   4.478E-01  2.500E-01
     LIQUID
  ** LIQUID#2
 Calculated                     2  equilibria
 Calculated                     2  equilibria
```

```
Phase region boundary   7 at:   4.478E-01  2.500E-01
    LIQUID
 ** LIQUID#2
Calculated                     45  equilibria

Phase region boundary   8 at:   4.478E-01  2.500E-01
    LIQUID
 ** LIQUID#2
Calculated.                     41  equilibria

Phase region boundary   9 at:   2.500E-01  4.478E-01
    LIQUID
 ** LIQUID#2
 ** LIQUID#3

Phase region boundary  10 at:   2.500E-01  4.478E-01
    LIQUID
 ** LIQUID#2
    LIQUID#3
Creating a new composition set LIQUID#4
Calculated                     31  equilibria

Phase region boundary  11 at:   2.500E-01  4.478E-01
    LIQUID
 ** LIQUID#2
    LIQUID#3
Calculated.                     15  equilibria

Phase region boundary  12 at:   1.816E-01  3.184E-01
    LIQUID
 ** LIQUID#2
    LIQUID#3
 ** LIQUID#4

Phase region boundary  13 at:   3.184E-01  3.184E-01
    LIQUID
    LIQUID#2
 ** LIQUID#3
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   3.184E-01  3.184E-01
    LIQUID
    LIQUID#2
 ** LIQUID#4
Calculated.                     14  equilibria

Phase region boundary  15 at:   4.478E-01  2.500E-01
 ** LIQUID
    LIQUID#2
 ** LIQUID#4

Phase region boundary  16 at:   4.478E-01  2.500E-01
    LIQUID#2
 ** LIQUID#4
Calculated.                     43  equilibria

Phase region boundary  17 at:   2.500E-01  5.217E-02
    LIQUID#2
 ** LIQUID#3
 ** LIQUID#4

Phase region boundary  18 at:   2.500E-01  5.217E-02
    LIQUID#2
    LIQUID#3
 ** LIQUID#4
Calculated                     20  equilibria

Phase region boundary  19 at:   2.500E-01  5.217E-02
    LIQUID#2
    LIQUID#3
 ** LIQUID#4
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  20 at:   2.500E-01  5.217E-02
    LIQUID#2
 ** LIQUID#3
Calculated.                     41  equilibria

Phase region boundary  21 at:   5.217E-02  2.500E-01
    LIQUID#2
 ** LIQUID#3
 ** LIQUID#4

Phase region boundary  22 at:   5.217E-02  2.500E-01
    LIQUID#2
 ** LIQUID#3
    LIQUID#4
Calculated                     20  equilibria

Phase region boundary  23 at:   5.217E-02  2.500E-01
    LIQUID#2
 ** LIQUID#3
    LIQUID#4
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  24 at:   5.217E-02  2.500E-01
    LIQUID#2
 ** LIQUID#4
Calculated.                     41  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   5.217E-02  2.500E-01
    LIQUID#2
    LIQUID#3
 ** LIQUID#4
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   2.500E-01  5.217E-02
    LIQUID#2
 ** LIQUID#3
    LIQUID#4
Calculated                     20  equilibria
```

```
 Phase region boundary  27 at:   2.500E-01  5.217E-02
     LIQUID#2
  ** LIQUID#3
     LIQUID#4
 Calculated.                     15  equilibria
 Terminating at known equilibrium

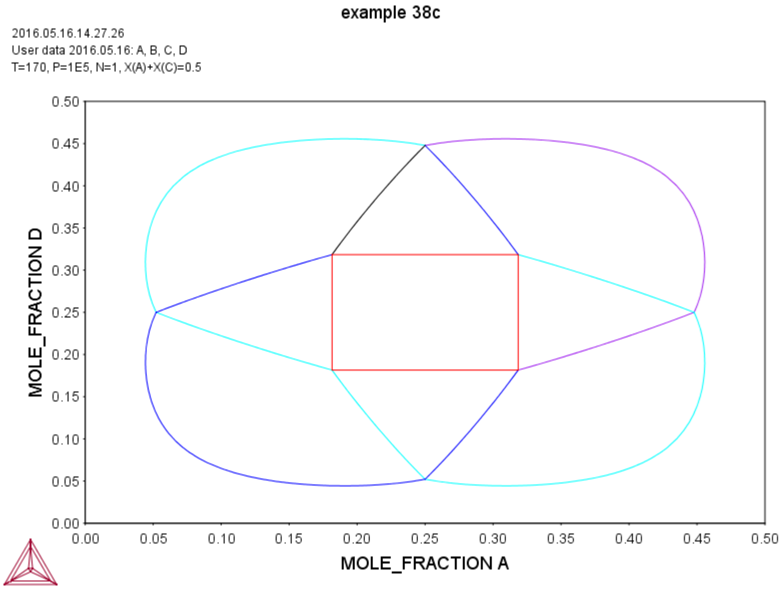
 Phase region boundary  28 at:   4.478E-01  2.500E-01
  ** LIQUID
     LIQUID#2
 Calculated.                     43  equilibria
 Terminating at known equilibrium

 Phase region boundary  29 at:   4.478E-01  2.500E-01
  ** LIQUID
     LIQUID#2
     LIQUID#4
 Calculated.                     15  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex38\tcex
 38c.POLY3
 CPU time for mapping                     1  seconds
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST:
POST: set-title example 38c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
 The composition set LIQUID#3 created from the store file
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex39

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex39.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ The  Calculation of the Reversible Carnot Cycle of Heat Engine
SYS: @@
SYS: @@
SYS: @@ The Reversible Carnot cycles are usually drawn schematically in lectures
SYS: @@ or text books and rarely understood by students. But by making use of
SYS: @@ a thermodynamic software system like Thermo-Calc and realistic data it
SYS: @@ is possible to calculate a reversible Carnot cycle of a heat engine
SYS: @@ and to relate it to different thermodynamic quantities.
SYS: @@ Some particular cases will be calculated and graphicaly presented in this
SYS: @@ example.
SYS: @@
SYS: @@
SYS: @@ One application of the Second Law is to the efficiencies of heat
SYS: @@ engines, pumps and refrigerators.
SYS: @@ Whenever there exists a difference of temperature, work can be
SYS: @@ produced - the principle of heat engines. The Gibbs energy also
SYS: @@ enables us to predict the maximum work that a process may achive.
SYS: @@
SYS: @@
SYS: @@ To illustrate how Thermo-Calc calculates the reversible Carnot cycle we
SYS: @@ will consider one mole of an ideal gas with two ficticious species A
SYS: @@ and A2.
SYS: set-log ex39,,,
SYS:
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: rei,,,,,
   ... the command in full is REINITIATE
GES: e-e a
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
GES: a-e-d a gas 10,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: e-sp A2 A2
   ... the command in full is ENTER_SPECIES
GES: e-ph gas g 1 A A2; N N
   ... the command in full is ENTER_PHASE
GES: @@ The Gibbs free energy for these specie could be described by
GES: @@ the general formula:  Gm= a +bT + cTlnT + dT2 +...+ RTln(P)
GES: @@
GES: @@ In order to calculate the Carnot cycle one has to give some numerical
GES: @@ values to the a, b, c, etc. constants of the Gm expression.
GES: @@ It is important to understand that the coefficients cannot be
GES: @@ chosen arbirarily, for example c should be negative as the heat capacity
GES: @@ at constant pressure, Cp = - T d2G/dT2 and thus Cp=-c-2dT must always be >0
GES: @@
GES: e-par g(gas,a) 298.15 6960-51*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,,
   ... the command in full is ENTER_PARAMETER
 G(GAS,A;0)-G(GAS,A;0)
GES: e-par g(gas,a2) 298.15 130670-38*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,,
   ... the command in full is ENTER_PARAMETER
 G(GAS,A2;0)- 2 G(GAS,A;0)
GES: l-d,,,,
   ... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE: User data 2016.05.16

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  1 A    GAS                       1.0000E+01  0.0000E+00  0.0000E+00


 SPECIES                                    STOICHIOMETRY
   1 A                                      A
   2 A2                                     A2



 GAS
    CONSTITUENTS: A,A2

      G(GAS,A;0)-G(GAS,A;0)  = +6960-51*T-17*T*LN(T)+R*T*LN(1E-05*P)
      G(GAS,A2;0)- 2 G(GAS,A;0)  = +130670-38*T-17*T*LN(T)+R*T*LN(1E-05*P)

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


GES:Hit RETURN to continue
GES: @@
GES: @@ The Carnot cycle diagram gives the pressure and volume for the
GES: @@ working media of a heat engine that operates between two temperatures
GES: @@ T1 and T2, T1>T2.
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@ The Carnot cycle will be calculated for T1=500 K (the temperature
POLY_3: @@ of the hot reservoire) and T2=400 K (the temperature of the cold
POLY_3: @@ reservoire)
POLY_3: ent var t1=500;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent var t2=400;
   ... the command in full is ENTER_SYMBOL
POLY_3: @@
```

```
POLY_3: @@ A Carnot cycle consists of four reversible stages:
POLY_3: @@
POLY_3: @@ Stage 1. Isothermal expansion at T1; the entropy change of the system is
POLY_3: @@ Q1/T1, where Q1 is the heat taken from the hot reservoire.
POLY_3: @@
POLY_3: @@
POLY_3: s-c t=t1 p=1e7 n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           137 grid points in             0 s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xn
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, P=1E7, N=1
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -5.22193E+04,  Enthalpy  1.54600E+04,  Volume  4.15725E-04

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       1.0000E+00  1.0000E+00 3.5061E-06 -5.2219E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  8.75433E-20
POLY_3:Hit RETURN to continue
POLY_3: @@ Set volume to 1 m3
POLY_3: s-c v
   ... the command in full is SET_CONDITION
Value /4.157255E-04/: 1
POLY_3: s-c n
   ... the command in full is SET_CONDITION
Value /1/: none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, P=1E7, V=1
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  2.40543E+03,  Mass in grams  2.40543E+04
 Total Gibbs energy -1.25610E+08,  Enthalpy  3.71880E+07,  Volume  1.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  8.75433E-20
POLY_3: s-c n
   ... the command in full is SET_CONDITION
Value /2405.433393/:
POLY_3: s-c p
   ... the command in full is SET_CONDITION
Value /10000000/: none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, N=2405.43, V=1
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  2.40543E+03,  Mass in grams  2.40543E+04
 Total Gibbs energy -1.25610E+08,  Enthalpy  3.71880E+07,  Volume  1.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  8.75433E-20
POLY_3: enter var ha=h;
   ... the command in full is ENTER_SYMBOL
POLY_3: enter var sa=s;
   ... the command in full is ENTER_SYMBOL
POLY_3: s-c s
   ... the command in full is SET_CONDITION
Value /325596.1064/: sa
POLY_3: s-c v=none
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
```

```
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, N=2405.43, S=SA
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  2.40543E+03,  Mass in grams  2.40543E+04
 Total Gibbs energy -1.25610E+08,  Enthalpy  3.71880E+07,  Volume  1.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  8.75433E-20
POLY_3:Hit RETURN to continue
POLY_3: show t,p,v,g,n,h,s
   ... the command in full is SHOW_VALUE
 T=500
 P=1E7
 V=1.
 G=-1.2561005E8
 N=2405.4334
 H=3.7188E7
 S=325596.11
POLY_3:Hit RETURN to continue
POLY_3: ent var ga=g;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent var pa=p;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent var va=v;
   ... the command in full is ENTER_SYMBOL
POLY_3: @@
POLY_3: @@
POLY_3: save tcex39a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: s-c s=204200
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 204000 205000,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           137 grid points in             0 s
    17 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    204200.
...OK

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04400E+05 .... OK
 Global test at  2.04650E+05 .... OK
 Global test at  2.04900E+05 .... OK
 Terminating at    205000.
 Calculated    35 equilibria

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04000E+05 .... OK
 Terminating at    204000.
 Calculated    11 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39a.POLY3
POLY_3: @@
POLY_3: @@
POLY_3: @@ Stage 2. Adiabatic expansion. No heat leaves the system, so the
POLY_3: @@ change in its entropy is zero. In the course of this expansion the
POLY_3: @@ temperature falls from T1 to T2, the temperature of cold reservoire.
POLY_3: @@
POLY_3: s-c s=205000
   ... the command in full is SET_CONDITION
POLY_3: s-c t=450
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 500,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           137 grid points in             0 s
    13 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
...OK

 Phase Region from    450.000     for:
     GAS
 Global test at  4.70000E+02 .... OK
 Global test at  4.95000E+02 .... OK
 Terminating at    500.000
 Calculated    23 equilibria

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Terminating at    400.000
 Calculated    23 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
```

```
 39a.POLY3
POLY_3: @@
POLY_3: @@ Stage 3. Isothermal compresion at T2. The heat Q2 is released to the
POLY_3: @@ cold reservoire, so the change in entropy of the system is -Q2/T2.
POLY_3: @@
POLY_3: s-c t=400
   ... the command in full is SET_CONDITION
POLY_3: s-c s=204200
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 204000 205000,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           137 grid points in              0 s
     8 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    204200.
...OK

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04400E+05 .... OK
 Global test at  2.04650E+05 .... OK
 Global test at  2.04900E+05 .... OK
 Terminating at    205000.
 Calculated    35 equilibria

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04000E+05 .... OK
 Terminating at    204000.
 Calculated    11 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39a.POLY3
POLY_3: @@
POLY_3: @@
POLY_3: @@ Stage 4. Adiabatic compression. No heat enters the system, so the change
POLY_3: @@ in entropy is zero. The temperature rises from T2 to T1.
POLY_3: @@
POLY_3: @@
POLY_3: s-c s=204000
   ... the command in full is SET_CONDITION
POLY_3: s-c t=450
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 500,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           137 grid points in              0 s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
...OK

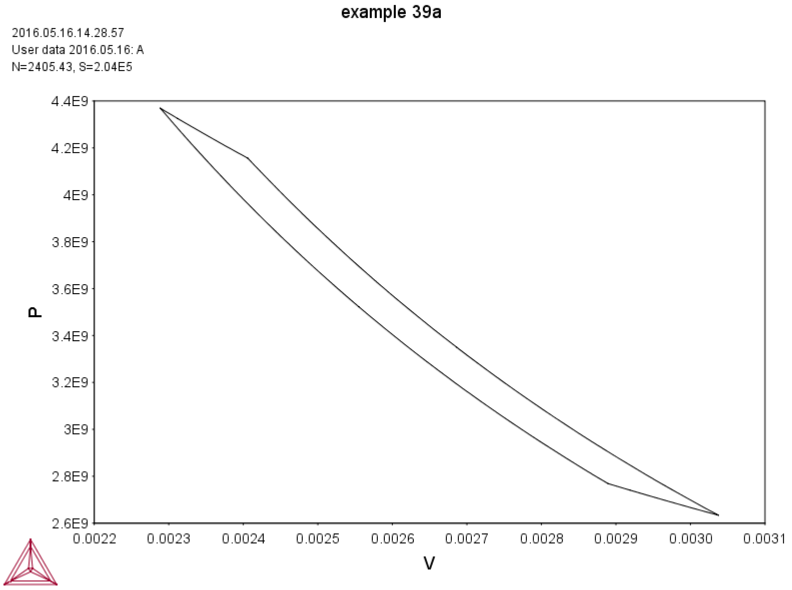
 Phase Region from    450.000     for:
     GAS
 Global test at  4.70000E+02 .... OK
 Global test at  4.95000E+02 .... OK
 Terminating at    500.000
 Calculated    23 equilibria

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Terminating at    400.000
 Calculated    23 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39a.POLY3
POLY_3:
POLY_3: post

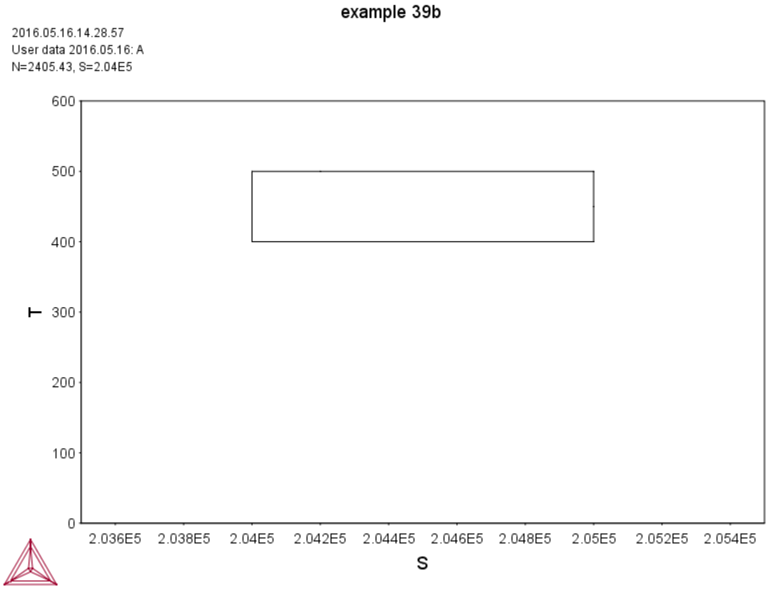
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:Plotformat
POST:
POST: s-p-f ##1,,,,,,,,,,,,
   ... the command in full is SET_PLOT_FORMAT
 CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ The efficiency E of an engine which uses a Carnot cycle is:
POST: @@
POST: @@ E=work performed/heat absorbed = W/Q1
POST: @@ If one plots the entropy versus temperature, one can calculate the
POST: @@ work performed just by calculating the area of the surface
POST: @@ depicted by the two squares and by making the difference between them.
POST: @@
POST: s-d-a x s
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n 0 600
   ... the command in full is SET_SCALING_STATUS
POST: s-s x n 203500 205500
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 39b
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@
POST: @@
POST: @@ The influence of the value of the temperature T1 (the temperature of the
POST: @@ hot reservoire) on the efficency of the Carnot cycle is important.
POST: @@ Therefor we will make an other calculation for T1=800 K and compare with
POST: @@ the one for T1=500 K (example 39a and b). T2=400 K in both cases.
POST: ba
   ... the command in full is BACK
POLY_3: read,,,
   ... the command in full is READ_WORKSPACES
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=T1, N=2405.43, S=SA
 DEGREES OF FREEDOM 0
POLY_3: s-c s=none
   ... the command in full is SET_CONDITION
POLY_3: s-c t=800  p=1e7 n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           137 grid points in             0 s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
```

```
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=800, P=1E7, N=1
 DEGREES OF FREEDOM 0

 Temperature    800.00 K (   526.85 C),  Pressure  1.000000E+07
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -9.41189E+04,  Enthalpy  2.05600E+04,  Volume  6.65161E-04

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 A                        1.0000E+00  1.0000E+00 7.1585E-07 -9.4119E+04 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  1.27812E-15
POLY_3: @@ Set volume to 1 m3
POLY_3: s-c v
   ... the command in full is SET_CONDITION
Value /6.651607999E-04/: 1
POLY_3: s-c n
   ... the command in full is SET_CONDITION
Value /1/: none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     7 ITS,  CPU TIME USED   0 SECONDS
POLY_3: s-c n
   ... the command in full is SET_CONDITION
Value /1503.395871/:
POLY_3: s-c p
   ... the command in full is SET_CONDITION
Value /10000000/: none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: enter var ha=h;
   ... the command in full is ENTER_SYMBOL
POLY_3: enter var sa=s;
   ... the command in full is ENTER_SYMBOL
POLY_3: s-c s
   ... the command in full is SET_CONDITION
Value /215509.7923/: sa
POLY_3: s-c v=none
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: show t,p,v,g,n,h,s
   ... the command in full is SHOW_VALUE
 T=800
 P=1E7
 V=1.
 G=-1.4149801E8
 N=1503.3959
 H=3.0909819E7
 S=215509.79
POLY_3:Hit RETURN to continue
POLY_3: save tcex39b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: s-c s=272000
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 270200 276200,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          137 grid points in             0 s
    53 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    272000.
...OK

 Phase Region from    272000.     for:
     GAS
 Global test at  2.73200E+05 .... OK
 Global test at  2.74700E+05 .... OK
 Global test at  2.76200E+05 .... OK
 Terminating at    276200.
 Calculated    31 equilibria

 Phase Region from    272000.     for:
     GAS
 Global test at  2.70800E+05 .... OK
 Terminating at    270200.
 Calculated    15 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39b.POLY3
POLY_3: s-c s=276200
   ... the command in full is SET_CONDITION
POLY_3: s-c t=750
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 800,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          137 grid points in             0 s
    13 ITS,  CPU TIME USED   0 SECONDS
```

```
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    750.000
...OK

 Phase Region from    750.000     for:
     GAS
 Terminating at    800.000
 Calculated     8 equilibria

 Phase Region from    750.000     for:
     GAS
 Global test at  6.70000E+02 .... OK
 Global test at  5.70000E+02 .... OK
 Global test at  4.70000E+02 .... OK
 Terminating at    400.000
 Calculated    38 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39b.POLY3
POLY_3: s-c t=400
   ... the command in full is SET_CONDITION
POLY_3: s-c s=270250
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 270200 276200,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           137 grid points in              0 s
     9 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    270250.
...OK

 Phase Region from    270250.     for:
     GAS
 Global test at  2.71450E+05 .... OK
 Global test at  2.72950E+05 .... OK
 Global test at  2.74450E+05 .... OK
 Global test at  2.75950E+05 .... OK
 Terminating at    276200.
 Calculated    43 equilibria

 Phase Region from    270250.     for:
     GAS
 Terminating at    270200.
 Calculated     4 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39b.POLY3
POLY_3: s-c s=270200
   ... the command in full is SET_CONDITION
POLY_3: s-c t=750
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 800,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           137 grid points in              0 s
    24 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    750.000
...OK

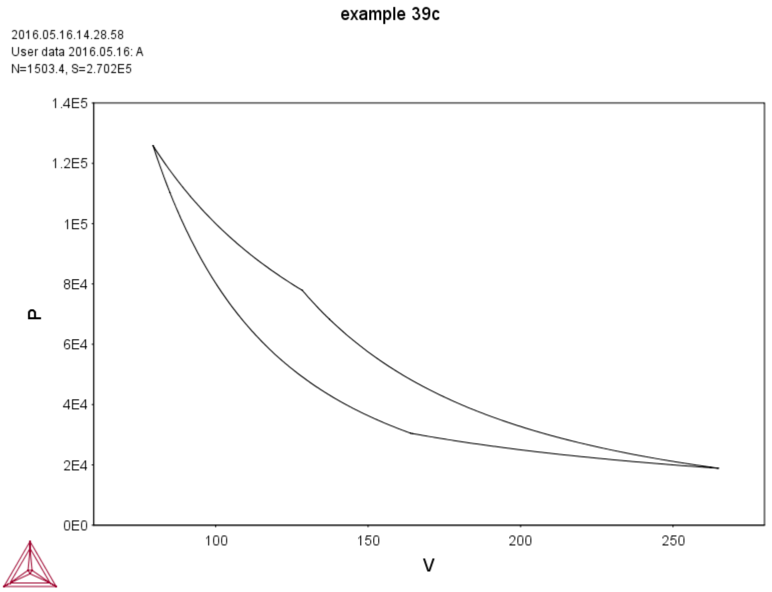
 Phase Region from    750.000     for:
     GAS
 Terminating at    800.000
 Calculated     8 equilibria

 Phase Region from    750.000     for:
     GAS
 Global test at  6.70000E+02 .... OK
 Global test at  5.70000E+02 .... OK
 Global test at  4.70000E+02 .... OK
 Terminating at    400.000
 Calculated    38 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39b.POLY3
POLY_3:
POLY_3: post

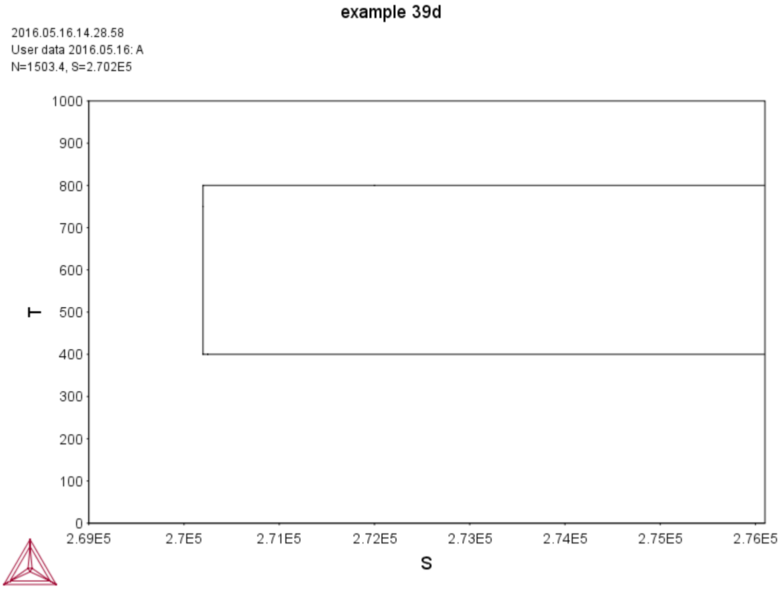
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-p-f ##1,,,,,,,,,
   ... the command in full is SET_PLOT_FORMAT
 CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39c
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: s-d-a x s
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 269000 276100
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1000
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 39d
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ The efficiency for high value of T1 temperature is almost double compared
POST: @@ with that one for low value of T1 temperature (compare example 39b with
POST: @@ example 39d).
POST: @@
POST: @@ Now we will calculate the Carnot cycle for some real systems. The most
POST: @@ well known engine is the steam engine.
POST: @@
POST: @@ The Carnot cycle for steam engine
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: go da
   ... the command in full is GOTO_MODULE
TDB_TCFE8: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
TDB_TCFE8: sw subdemo
   ... the command in full is SWITCH_DATABASE
 Current database: Substance Demo Database

 VA                      /-  DEFINED
TDB_SUBDEMO: def-sp h2o1
   ... the command in full is DEFINE_SPECIES
 H2O1  DEFINED
TDB_SUBDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
 GAS:G       :H2O1:
 H2O1_L      :H2O1:
TDB_SUBDEMO: get
```

```
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
  'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
 -OK-
TDB_SUBDEMO: @@ patch
TDB_SUBDEMO: go g-e-s
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: li-st,,,,,
   ... the command in full is LIST_STATUS
 GAS CONSTANT IN USER ENERGY UNITS:      8.31451000E+00
 1 BAR IN USER PRESSURE UNITS:           1.00000000E+05
 CURRENT VALUE OF TEMPERATURE (KELVIN):          298.15
 CURRENT VALUE OF PRESSURE (PASCAL):     1.00000000E+05

 CURRENT NUMBER OF ELEMENT     4

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00 80000000
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00 80000000
  1 H    1/2_MOLE_H2(GAS)          1.0079E+00  4.2340E+03  6.5285E+01 08000000
  2 O    1/2_MOLE_O2(GAS)          1.5999E+01  4.3410E+03  1.0252E+02 08000000

 CURRENT NUMBER OF PHASE       2

 PHASE                          STATUS   SUBLATTICES
   1 GAS                        88200000     1
   2 H2O1_L                     82200000     1

 CURRENT NUMBER OF SPECIES     4

 SPECIES                                    STOICHIOMETRY
   1 H                           80800000   H
   2 H2O1                        00000000   H2O1
   3 O                           80800000   O
   4 VA                          81800000   VA

GES: @@ patch
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 H2O1_L                  ENTERED      0.000000E+00    0.000000E+00
 GAS                     ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY_3: c-st p h2o_l=sus
   ... the command in full is CHANGE_STATUS
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 GAS                     ENTERED      0.000000E+00    0.000000E+00
 SUSPENDED PHASES:
 H2O1_L
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY_3: @@ The Carnot cycle will be calculated for T1=350 K and T2=450 K
POLY_3: @@
POLY_3: s-c t=380 p=1e5 n=100 ac(o)=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated             1 grid points in             0 s
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature    380.00 K (   106.85 C),   Pressure  1.000000E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.04643E+07,  Enthalpy -7.96861E+06,  Volume  1.05317E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 2.6556E-22 -1.5697E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                           Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
```

```
 H2O1  1.00000E+00
POLY_3: s-c p=none
   ... the command in full is SET_CONDITION
POLY_3: s-c s
   ... the command in full is SET_CONDITION
Value /6567.729231/: 6100
POLY_3: s-c t=350
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated              1 grid points in              0 s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 T=350, N=100, AC(O)=1, S=6100
 DEGREES OF FREEDOM 0

 Temperature    350.00 K (    76.85 C),  Pressure  3.863619E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.01376E+07,  Enthalpy -8.00259E+06,  Volume  2.51067E-01

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 2.0244E-23 -1.5206E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY_3: @@ step in S with t=350
POLY_3: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex39c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
...OK

 Phase Region from    6100.00     for:
     GAS
 Global test at  6.30000E+03 .... OK
 Global test at  6.55000E+03 .... OK
 Global test at  6.80000E+03 .... OK
 Terminating at    7000.00
 Calculated    39 equilibria

 Phase Region from    6100.00     for:
     GAS
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39c.POLY3
POLY_3:
POLY_3:
POLY_3: read,,,,
   ... the command in full is READ_WORKSPACES
POLY_3: s-c s=6000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated              1 grid points in              0 s
     8 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ step in T with S=6000
POLY_3: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    350.000
...OK

 Phase Region from    350.000     for:
     GAS
 Global test at  3.70000E+02 .... OK
 Global test at  3.95000E+02 .... OK
 Global test at  4.20000E+02 .... OK
 Global test at  4.45000E+02 .... OK
 Terminating at    450.000
 Calculated    43 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39c.POLY3
POLY_3:
POLY_3: read,,,,
   ... the command in full is READ_WORKSPACES
POLY_3: s-c t=450
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated              1 grid points in              0 s
     9 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Step in S with t=450
POLY_3: @@@@
POLY_3: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
...OK
```

```
 Phase Region from    6100.00     for:
     GAS
 Global test at  6.30000E+03 .... OK
 Global test at  6.55000E+03 .... OK
 Global test at  6.80000E+03 .... OK
 Terminating at    7000.00
 Calculated    39 equilibria

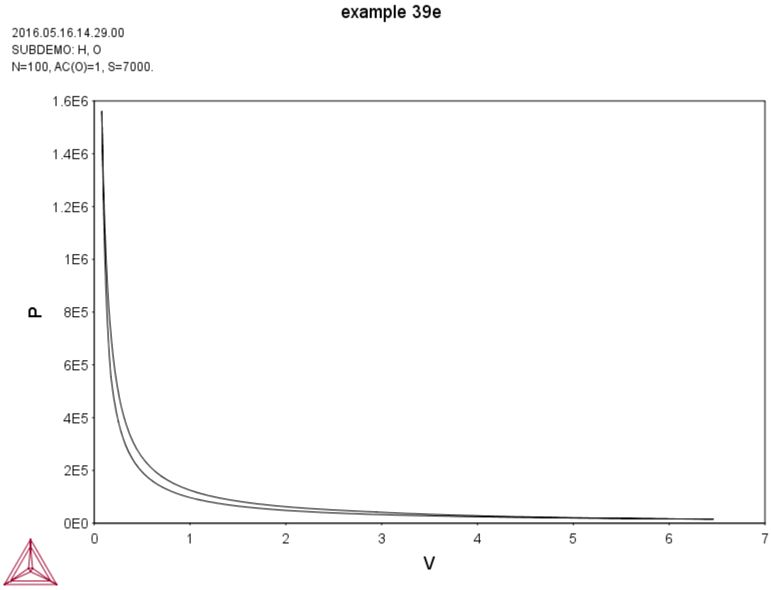
 Phase Region from    6100.00     for:
     GAS
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39c.POLY3
POLY_3:
POLY_3: s-c s=7000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated              1 grid points in             0 s
    42 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Step in T with S=7000
POLY_3: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
...OK

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Global test at  3.80000E+02 .... OK
 Global test at  3.55000E+02 .... OK
 Terminating at    350.000
 Calculated    43 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39c.POLY3
POLY_3:
POLY_3: post

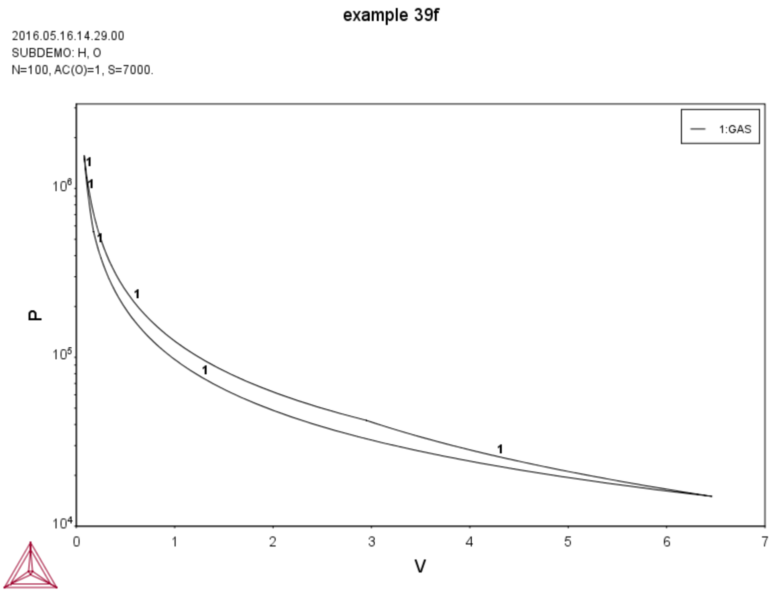
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

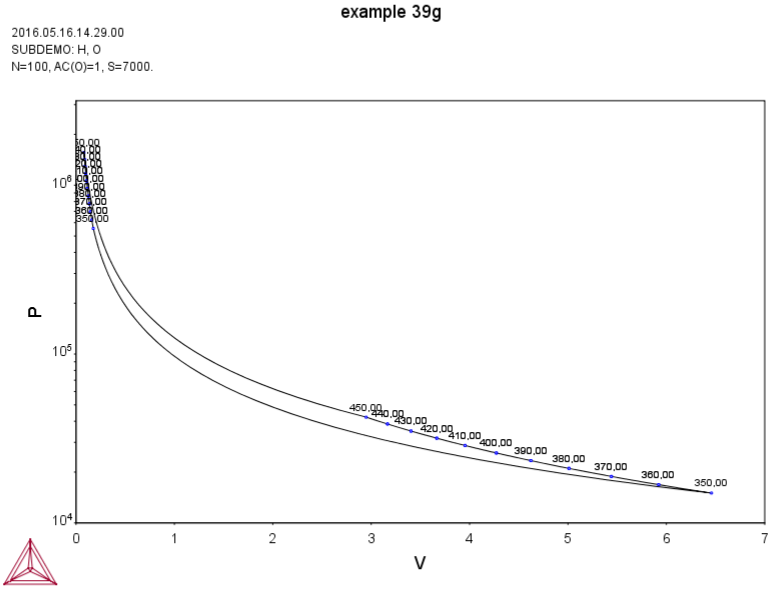
POST: s-p-f ##1,,,,,,,,
   ... the command in full is SET_PLOT_FORMAT
 CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39e
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39f
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ It is a bit difficult to distinguish from the calculated diagram,
POST: @@ example 39e, where the adiabatic expansion and compresion start.
POST: @@ Therefore it is good to plot on the same diagram also the temperature.
POST: @@
POST: s-d-a z t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab none
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39g
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@
POST: @@ With Thermo-Calc one may also calculate the Carnot cycle  for real systems
POST: @@ and also include phase transformations.
POST: @@
POST: @@ Trying a Carnot cycle for water - it shows the case with H2O_liquid
POST: @@ to gas phase transformation. In the calculations the volum of the liquid
POST: @@ water was ignored.
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: go da
   ... the command in full is GOTO_MODULE
TDB_SUBDEMO: rej sys
   ... the command in full is REJECT
 VA                        /-   DEFINED
 REINITIATING GES5 .....
TDB_SUBDEMO: sw subdemo
   ... the command in full is SWITCH_DATABASE
TDB_SUBDEMO: def-sp h2o1
   ... the command in full is DEFINE_SPECIES
 H2O1   DEFINED
TDB_SUBDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
 GAS:G        :H2O1:
 H2O1_L       :H2O1:
TDB_SUBDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
```

```
 FUNCTIONS ....

 List of references for assessed data

  'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
  'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
 -OK-
TDB_SUBDEMO: @@ patch
TDB_SUBDEMO: go g-e-s
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: li-st,,,,,
   ... the command in full is LIST_STATUS
 GAS CONSTANT IN USER ENERGY UNITS:      8.31451000E+00
 1 BAR IN USER PRESSURE UNITS:           1.00000000E+05
 CURRENT VALUE OF TEMPERATURE (KELVIN):          298.15
 CURRENT VALUE OF PRESSURE (PASCAL):     1.00000000E+05

 CURRENT NUMBER OF ELEMENT     4

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00 80000000
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00 80000000
  1 H    1/2_MOLE_H2(GAS)          1.0079E+00  4.2340E+03  6.5285E+01 08000000
  2 O    1/2_MOLE_O2(GAS)          1.5999E+01  4.3410E+03  1.0252E+02 08000000

 CURRENT NUMBER OF PHASE       2

 PHASE                          STATUS    SUBLATTICES
   1 GAS                        88200000     1
   2 H2O1_L                     82200000     1

 CURRENT NUMBER OF SPECIES     4

 SPECIES                                       STOICHIOMETRY
   1 H                           80800000    H
   2 H2O1                        00000000    H2O1
   3 O                           80800000    O
   4 VA                          81800000    VA

GES: @@ patch
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 H2O1_L                   ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY_3: c-st p h2o_l=e 0
   ... the command in full is CHANGE_STATUS
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 H2O1_L                   ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY_3: s-c t=380 p=1e5 n=100 ac(o)=1
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated              2 grid points in              0 s
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature    380.00 K (   106.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.04643E+07,  Enthalpy -7.96861E+06,  Volume  1.05317E+00

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 H                        6.6667E+01  6.6667E-01 2.6556E-22 -1.5697E+05 SER
 O                        3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY_3: s-c p=none
   ... the command in full is SET_CONDITION
POLY_3: s-c s
   ... the command in full is SET_CONDITION
```

```
Value /6567.729231/: 6100
POLY_3: s-c t=350
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated             2 grid points in             0 s
    36 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 T=350, N=100, AC(O)=1, S=6100
 DEGREES OF FREEDOM 0

 Temperature    350.00 K (    76.85 C),  Pressure  4.130269E+04
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.03545E+07,  Enthalpy -8.21947E+06,  Volume  1.98337E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 6.6188E-24 -1.5532E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 8.4450E+01, Mass 5.0711E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00

 H2O1_L                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.5550E+01, Mass 9.3379E+01, Volume fraction 0.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY_3: @@ step in S with t=350
POLY_3: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex39d y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
...OK

 Phase Region from    6100.00     for:
     GAS
     H2O1_L
 Global test at  6.30000E+03 .... OK
 Global test at  6.55000E+03 .... OK
 Global check of removing phase at  6.71967E+03
 Calculated    27 equilibria

 Phase Region from    6719.67     for:
     GAS
 Global test at  6.90000E+03 .... OK
 Terminating at    7000.00
 Calculated    15 equilibria

 Phase Region from    6100.00     for:
     GAS
     H2O1_L
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39d.POLY3
POLY_3:
POLY_3: read,,,,
   ... the command in full is READ_WORKSPACES
POLY_3: s-c s=6000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated             2 grid points in             0 s
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ step in T with S=6000
POLY_3: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    350.000
...OK

 Phase Region from    350.000     for:
     GAS
     H2O1_L
 Global test at  3.70000E+02 .... OK
 Global test at  3.95000E+02 .... OK
 Global test at  4.20000E+02 .... OK
 Global test at  4.45000E+02 .... OK
 Terminating at    450.000
 Calculated    43 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39d.POLY3
POLY_3:
POLY_3: read,,,,
   ... the command in full is READ_WORKSPACES
POLY_3: s-c t=450
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated             2 grid points in             0 s
    12 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Step in S with t=450
POLY_3: @@
POLY_3: s-a-v 1 s 6000 7000,,,,
```

```
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
...OK

 Phase Region from    6100.00     for:
     GAS
     H2O1_L
 Global check of removing phase at  6.16203E+03
 Calculated     5 equilibria

 Phase Region from    6162.03     for:
     GAS
 Global test at  6.35000E+03 .... OK
 Global test at  6.60000E+03 .... OK
 Global test at  6.85000E+03 .... OK
 Terminating at    7000.00
 Calculated    37 equilibria

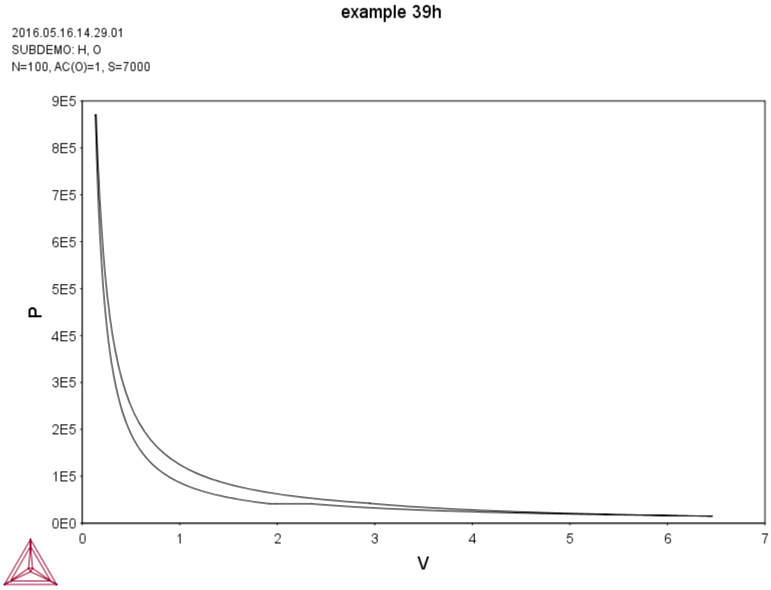
 Phase Region from    6100.00     for:
     GAS
     H2O1_L
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39d.POLY3
POLY_3:
POLY_3: s-c s=7000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated             2 grid points in             0 s
    40 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Step in T with S=7000
POLY_3: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
...OK

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Global test at  3.80000E+02 .... OK
 Global test at  3.55000E+02 .... OK
 Terminating at    350.000
 Calculated    43 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
 39d.POLY3
POLY_3:
POLY_3: post

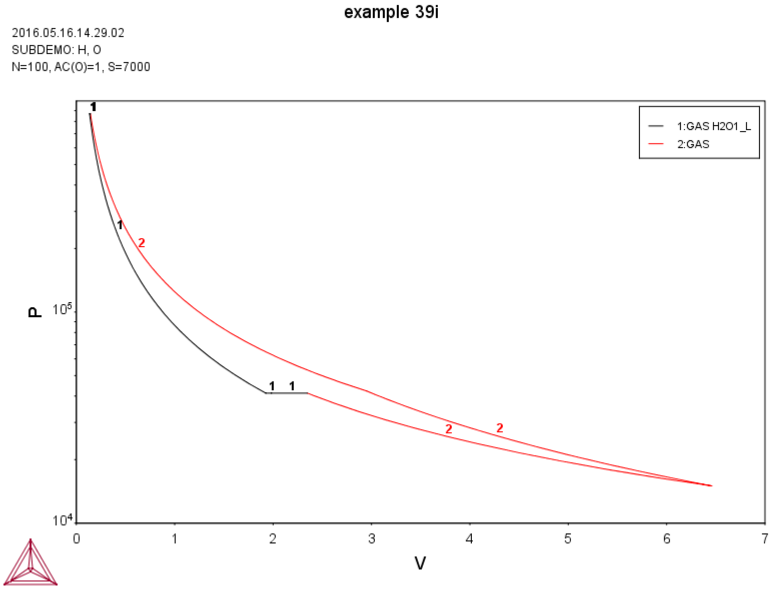
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

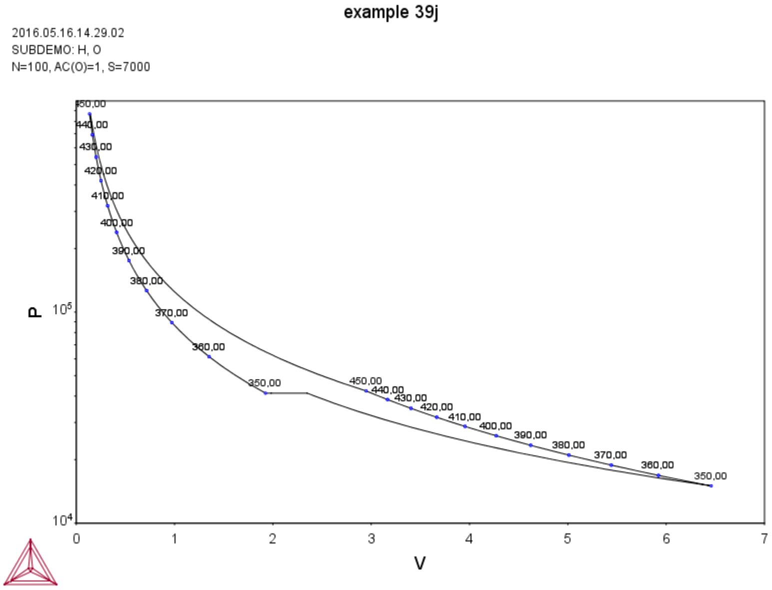
POST: @@ The cycle shows the constant pressure at phase transformation.
POST: s-p-f ##1,,,,,,,,,
   ... the command in full is SET_PLOT_FORMAT
 CURRENT DEVICE: TC-UNITE Driver
POST:
POST: @@ To get a better understanding of this process it is now possible to plot
POST: @@ the cycle using any set of thermodynamic state variables.
POST: @@ Thus, from the pressure-volume-temperature diagram, example 39g, it is
POST: @@ possible to see the temperature variation on the two adiabatical stages
POST: @@ of the Carnot cycle.
POST: @@ The cycle shows the constant pressure at phase transformation.
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39h
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



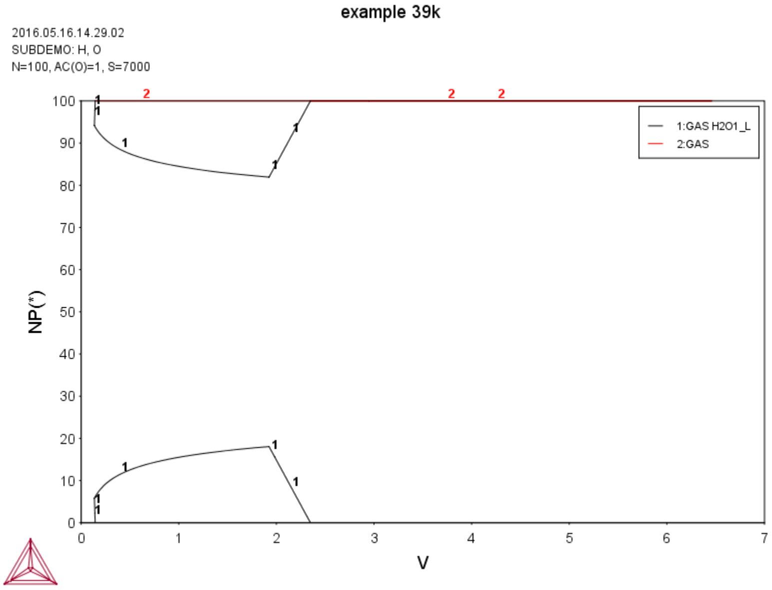
```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-tit example 39i
   ... the command in full is SET_TITLE
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



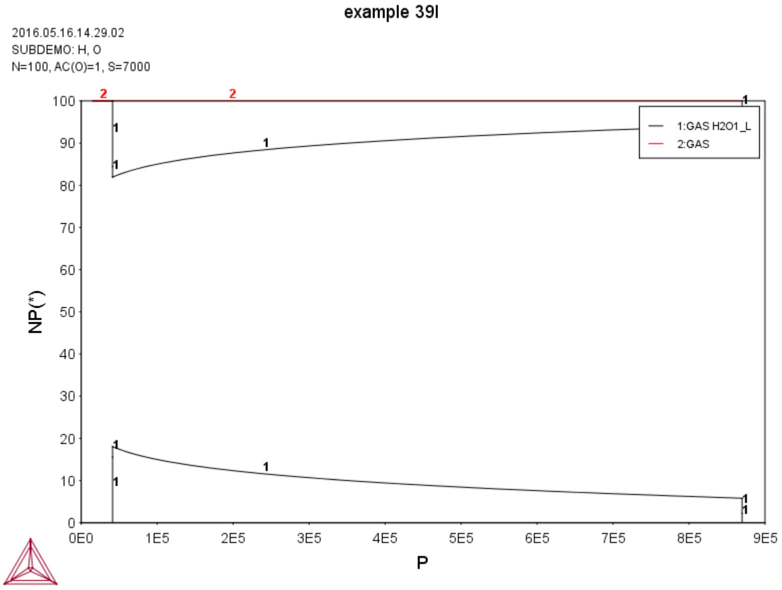
```
POST:
POST:Hit RETURN to continue
POST: s-d-a z t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab none
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39j
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



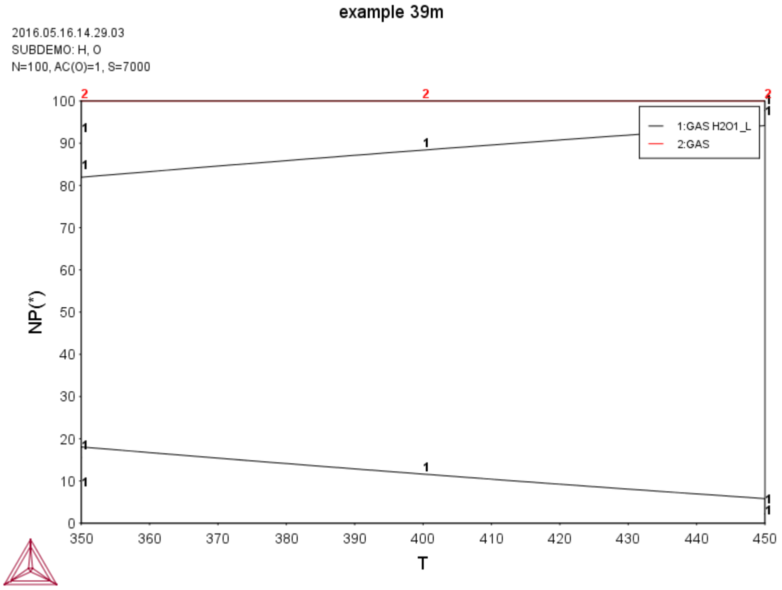
```
POST:
POST:Hit RETURN to continue
POST: @@ Also interesting seems to plot the amount of phases versus volume. One
POST: @@ could get information about both the kind and amount of phases which
POST: @@ fill up a certain volume.
POST: s-d-a z none
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*),,,
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty y,,,
   ... the command in full is SET_AXIS_TYPE
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39k
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



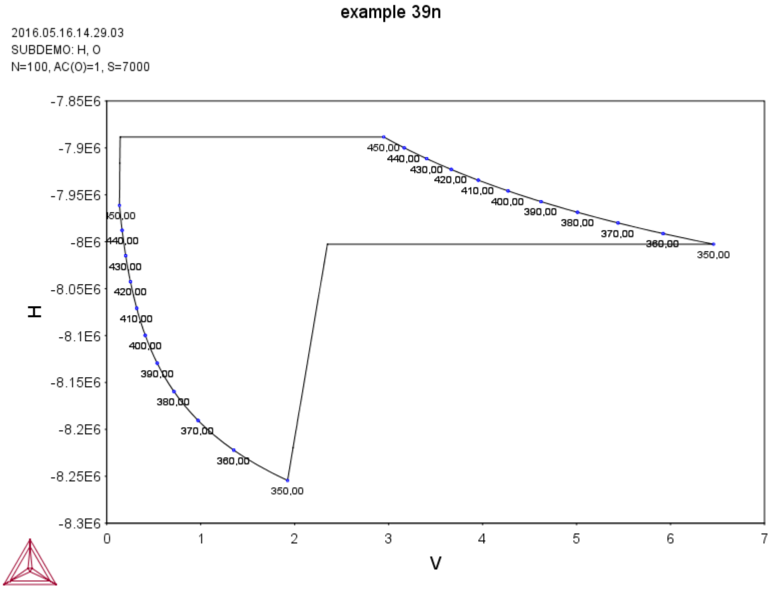
```
POST:
POST:Hit RETURN to continue
POST: @@ Next diagram shows the amount of phases versus pressure. It gives important
POST: @@ information on the phase transformation pressure and on the ratio
POST: @@ between the two phases in equilibrium at a certain pressure.
POST: @@
POST: s-d-a x p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39l
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



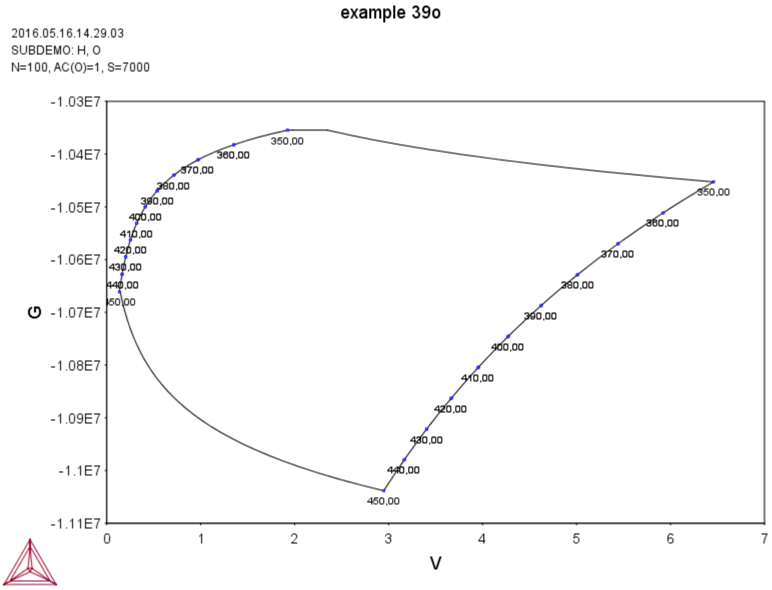
```
POST:
POST:Hit RETURN to continue
POST: @@ By ploting the amount of phases versus temperature, example 39k, it is
POST: @@ possible to know the phase transformation temperature and also the ratio
POST: @@ between the two phases in equilibrium at a certain temperature.
POST: @@
POST: s-d-a x t
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39m
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ The enthalpy and Gibbs energy for the Carnot cycle could also be
POST: @@ ploted using the same calculation but a different set for diagram axis.
POST: @@ Note the important drop of the enthalpy at the phase transformation
POST: @@ point, example 39l.
POST: s-lab none
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y h
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z t
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39n
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y g
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39o
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex40-TCEX40

```
About Stockholm, Sweden

 Software  (build 9597) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Tue May 17 19:06:04 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex40\TCEX40.TCM"SYS:
SYS:SYS: set-echo
SYS:
SYS: set-log TCEX40.LOG
Heading: Pourbaix Diagram Calculations through the advanced POURBAIX module
SYS:
SYS: @@
SYS: @@ TCEX40: Thermo-Calc 4.0 (Console Mode) Standard Example No 40
SYS: @@ ******* ============================================================
SYS: @@   Copyright: Thermo-Calc Software AB, Stockholm, Sweden
SYS: @@   Developer: Dr. Pingfang Shi, Thermo-Calc Software AB
SYS: @@   Date:      2014-05-18 (revision)
SYS: @@
SYS: @@ Pourbaix Diagram Calculations through the advanced POURBAIX module
SYS: @@ ********************************************************************
SYS: @@    * Using PAQ2 or PAQS2 database;
SYS: @@    * For the Fe-H2O-NaCl heterogeneous interaction systems
SYS: @@
SYS: @@ List of all the TC4-CM_Ex40 examples related to the POURBAIX module:
SYS: @@ --------------------------------------------------------------------
SYS: @@  TCEX40:
SYS: @@    * With the Main Option 1
SYS: @@    * Using the Single-Database Option, i.e., retrieving data from
SYS: @@        the PAQ2 [TCS Public Aqueous Solution (SIT) Database, v2.4;
SYS: @@        using the SIT aqueous solution model] or PAQS2 [TCS Public
SYS: @@        Aqueous Solution Database, v2.4; using the Complete Revised
SYS: @@        HKF aqueous solution model]; both of which contain an AQUEOUS
SYS: @@        solution phase and REF_ELECTRODE phase (as a reference for
SYS: @@        electron in aqueous electrolyte systems), as well as some
SYS: @@        data for various solid phases (solution or stoichiometric)
SYS: @@        and gaseous mixture phase. The PAQ2 and PAQS2 are specially
SYS: @@        designed for demonstrations of calculations of the so-called
SYS: @@        Pourbaix diagrams (i.e., pH-Eh plots) and other types of
SYS: @@        phase diagrams or property diagrams in some aqueous-bearing
SYS: @@        multicomponent heterogeneous interaction systems within the
SYS: @@        limited chemical framework of Fe-Co-Cr-Ni-C-N-S-H2O-NaCl,
SYS: @@        via the Single-Database Option in the advanced POURBAIX
SYS: @@        module or through the normal TDB-GES-PLOY-POST routine.
SYS: @@    * By reading a saved POURBAIX.POLY3 file (or renamed as another
SYS: @@        name), one can further run the following Main Options:
SYS: @@          Main Option 2 for plotting many other property diagrams
SYS: @@                          of the calculated interaction system;
SYS: @@          Main Option 3 for making another POURBAIX calculation
SYS: @@                          of the same chemical system but under
SYS: @@                          a different P-T-X condition;
SYS: @@          Main Option 4 for making a POLY3 STEPPING calculation
SYS: @@                          of the same chemical system but varied
SYS: @@                          with only one independent variable;
SYS: @@        ** The Main Options 2, 3 and 4 are not illustrated in this
SYS: @@           TCEX40 example.
SYS: @@
SYS: @@  Note that five more examples (TCEX40A, TCEX40B, TCEX40C, TCEX40D
SYS: @@     and TCEX40E) are also provided to demonstrate various options
SYS: @@     and features in the POURBAIX module and to show more advanced
SYS: @@     applications of the TCAQ2 and AQS2 aqueous solution databases
SYS: @@     [in the Multiple-Database Option, i.e., with appended data
SYS: @@     from the SSOL5 and SSUB5 databases].
SYS: @@
SYS: @@ --------------------------------------------------------------------
SYS: @@ In this Standard Example (TCEX40):
SYS: @@ ===================================
SYS: @@   The Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous
SYS: @@     solution at 25C and 1 bar is automatically calculated and
SYS: @@     plotted.
SYS: @@
SYS: @@   A so-called Pourbaix diagram is actually a phase diagram with
SYS: @@     independently-varied acidity (pH) and electropotential (Eh),
SYS: @@     for a heterogeneous interaction system at a certain bulk
SYS: @@     composition (that is by default always set as 1 kg of water
SYS: @@     dissolving a specified amount of metals and other solutes),
SYS: @@     under a defined temperature and pressure condition.
SYS: @@
SYS: @@   Some other diagrams, along various phase boundaries for the
SYS: @@     same interactions resulted from the same POURABIX Module
SYS: @@     calculation, are also plotted.
SYS: @@ --------------------------------------------------------------------
SYS: @@
SYS:
SYS:
SYS: @@... Now, let's start using the advanced POURBAIX Module:
SYS: @@
SYS: go pour
   ... the command in full is GOTO_MODULE

                 WELCOME TO THE POURBAIX MODULE
                 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
          for Quick Calculations of Pourbaix Diagrams
          ===========================================

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                     Norra Stationsgatan 93
                   SE-113 47 Stockholm, Sweden

                   (Version 7.0,  Mar. 2014)

Need any instruction on the POURBAIX module? /N/: ?

   IMPORTANT NOTES for Calculating a POURBAIX Diagram:
   ------------------------------------------------------------
```

1) The so-called Pourbaix diagram is actually a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (Eh, as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modelled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).
2) One must have at least a database containing an AQUEOUS solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc database spectrum, or be chosen from an appropriate USER-specified database (it must be in the Thermo-Calc TDB format).
3) Due to the restrictions of aqueous solution model used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ) or AQS (PAQS) for AQUEOUS solution phase. Among others, one should keep in mind the following regulations:
   * The ELECTRON is defined as an special element (ZE) and as the only constituent in its reference phase REFERENCE_ELECTRODE (for determining the electro-potential that is defined as Eh with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;
   * The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;
   * The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.
4) Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H2O1, O2 and H2; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!
5) All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a GASeous mixture phase, a REF_ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above). Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the TCAQ or AQS as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended). Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAl, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for GASeous mixture phase and for varous solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.
6) The current advanced POURBAIX-Module has been designed and developed in an efficient and effective way that it only requires the user to just answer some simple and necessary questions, rather than to go through basic modules (i.e., TDB, GES5, POLY3 and POST) and type the ordinary command-lines. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.
7) The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-PLOY3-POST calculation.

Enforce a PAUSE after plotting when running a MACRO? /N/: ?

Whenever running a Thermo-Calc MACRO (TCM) file, you may prefer to have a PAUSE after a specific diagram has been plotted on SCREEN, for the multiple purposes of efficiently and easily manipulating the plotted diagram directly on the traditional TC-Graph window or Java-based TC-UNITE window, such as:

* Printing it (of EMF/PS format) on connected printer(s);
* Converting it (of EMF format) to (PDF) graphical files;
* Saving it as an EMF graphical file;
* Dumping it as a PNG or BMP graphical file;
* Setting background colour for the current diagram and for all the sequential plots;
* Setting default font/size for all the sequential plots;
* Changing plotting Layers for all the sequential plots.

```
    If no PAUSE is enforced, the POURBAIX Module will be going
    through all the sequential command-lines (answers) in the
    same POURBAIX session or till the SET_INTERACTIVE_MODE line
    in the MACRO file has been reached.

    ----------------------------------------------------------
    ** By Y(y), a PAUSE is always enforced after each diagram;
    ** By N(n), no PAUSE will be enforced at any point at all.
    ----------------------------------------------------------
    Please then press <RETURN> at the PAUSE for continuation!

Enforce a PAUSE after plotting when running a MACRO? /N/: y

    ----------------------------------------------------------
   |                                                          |
   |  1. Start a completely new POURBAIX diagram calculation  |
   |  2. Open an old file & plot other property diagrams      |
   |  3. Open an old file & make another POURBAIX calculation |
   |  4. Open an old file & make another STEPPING calculation |
   |                                                          |
    ----------------------------------------------------------

Select option /1/: ?

   One of the four options (1/2/3/4) should be entered here:

    1 -- Make a completely new POURBAIX diagram calculation
           and automatically plot a pH-Eh diagram.
              i.e., define a new chemical system;
                    specify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.

    2 -- Open an existing POLY3 file created by POURBAIX Module
            (from a previous POURBAIX calculation Option 1 or 3
              or  a previous STEPPING calculation Option 4),
           and just selectively plot other property diagrams.
              i.e., open the old GES and POLY3 workspaces;
                    plot pH-Eh or various property diagrams.

    3 -- Open an existing POLY3 file created by POURBAIX Module
           and make another POURBAIX diagram calculation.
              i.e., open the old GES and POLY3 workspaces;
                    adopt the defined chemical system;
                    modify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.

    4 -- Open an existing POLY3 file created by POURBAIX Module
            (from a previous POURBAIX calculation Option 1 or 3
              or  a previous STEPPING calculation Option 4),
           and make a normal STEPPING calculation.
              i.e., open the old GES and POLY3 workspaces;
                    adopt the defined chemical system;
                    specify one of the T-P-X conditions
                             as the stepping variable;
                    calculate the initial equilibria;
                    perform the stepping calculation;
                    plot various property diagrams.

Select option /1/: 1

    1 -- Make a completely new POURBAIX diagram calculation
           and automatically plot a pH-Eh diagram.
              i.e., define a new chemical system;
                    specify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: ?

    You may optionally choose to ignore the GAS mixture phase
    on a calculated/plotted Pourbaix diagram. However, such a
    plot is actually not a complete Pourbaix diagram, due to
    that the thermodynamically-stable phase boundaries between
    the AQUEOUS solution phase and GAS mixture phase will not
    be calculated at all.

    ----------------------------------------------------------
    ** By Y(y), GAS mixture phase shall be always considered;
    ** By N(n), GAS mixture phase will be completely ignored.
    ----------------------------------------------------------

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: Y

Use single database? /Y/: Y
Combined Database: /PAQ2/: PAQ2
 THERMODYNAMIC DATABASE module
 Current database: Public Aqueous Soln (SIT) TDB v2.4

 H                        O                        ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                 DIAMOND_A4               FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                 CUB_A13                  CHI_A12
 FE4N                     FECN_CHI  REJECTED
 CEMENTITE                M23C6                    M7C3
 M5C2                     M3C2                     KSI_CARBIDE
 PI  REJECTED
 FE3C                     NI3C                     CR3C2
 CR7C3                    CR23C6  REJECTED
 COCO3                    FECO3                    NAHCO3
 NA2CO3                   NA2CO3_S2                NICO3
 CRC6O6  REJECTED
 CO3N                     CRN                      CR2N
 FE2N                     NI3N  REJECTED
 NANO2                    NANO2_S2                 NANO3
   REJECTED
 COCL2                    CRCL2                    CRCL3
 FECL2                    FECL3                    NICL2
   REJECTED
```

```
 FECLO                    NACLO4                   NACLO4_S2
   REJECTED


 DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION:
 ==============================================================
 Normally a POURBAIX diagram and related equilibrium property
 in a heterogeneous interaction system are calculated under a
 certain bulk composition which is usually 1 kg of water with
 defined amounts of dissolving solute substances. The solutes
 may either be completely dissolved into the aqueous solution,
 or be partially dissolved and simultaneously form some solid
 phases.

 CHEMICAL SYSTEM (ELEMENTS):
    Default defined elements  (solvent  H2O):     H  &  O
            and specially assigned ZE(electron) & VA(vacancy).
    Prompt specified elements (solutes  ELEM):
            Fe  Ni  Co  Cr  C   N   S   Na  Cl
 INITIAL BULK COMPOSITION:
    Default defined composition  (solvent):    1.0 kg of H2O
    Prompt specified composition (solutes):    x mole of ELEM
 --------------------------------------------------------------
 Notes: For accepting a default value, just RETURN at prompt;
        For changing to a specific value, enter it at prompt.

 ==============================================================
 IMPORTANT NOTE for Entering Solutes in Chemical Formulas:
   First element letter in UPPER case, and second lower case!
     such as  NaCl  CO2  CoCl3  Fe0.93S  NaSO4-1  H2SO4
 --------------------------------------------------------------
   Mass of Water (weight) = 1 kg

   First solute: Fe
     Molality of Fe (mole/kg) /.001/: .001
   Second solute: NaCl .1
   Next solute:

 ------------------------------------------------------------
 Defined chemical system and initial bulk composition:
    Note: Solutes have been split up into chemical elements
          and their mole numbers. If confirmed, the POURBAIX
          Module will, in further steps, count the initial
          bulk composition in terms of chemical elements.
 ------------------------------------------------------------
         H2O           1.00000000       kg
         ZE           (specially assigned)
          FE          0.1000000000E-02  mole
          CL          0.1000000000E+00  mole
          NA          0.1000000000E+00  mole

Confirm defined system and initial bulk composition? /Y/: Y


RETRIEVE THERMODYNAMIC DATA FROM THE DATABASE:  PAQ2

 H                        O                        ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                 DIAMOND_A4               FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                 CUB_A13                  CHI_A12
 FE4N                     FECN_CHI  REJECTED
 CEMENTITE                M23C6                    M7C3
 M5C2                     M3C2                     KSI_CARBIDE
 PI  REJECTED
 FE3C                     NI3C                     CR3C2
 CR7C3                    CR23C6  REJECTED
 COCO3                    FECO3                    NAHCO3
 NA2CO3                   NA2CO3_S2                NICO3
 CRC6O6  REJECTED
 CO3N                     CRN                      CR2N
 FE2N                     NI3N  REJECTED
 NANO2                    NANO2_S2                 NANO3
   REJECTED
 COCL2                    CRCL2                    CRCL3
 FECL2                    FECL3                    NICL2
   REJECTED
 FECLO                    NACLO4                   NACLO4_S2
   REJECTED
 REINITIATING GES5 .....
 FE  DEFINED
 CL  DEFINED
 NA  DEFINED
 /-  DEFINED


 This database has following phases for the defined system

 AQUEOUS:A                 REF_ELECTRODE             GAS:G
 FCC_A1                    BCC_A2                    HCP_A3
 HALITE                    WUSTITE                   MAGNETITE
 HEMATITE                  FE2O3_GAMMA               FEO2H2
 FEO3H3                    FEOOH                     FE2O2O2H2
 NAO2                      NA2O                      NA2O_S2
 NA2O_S3                   NA2O2                     NA2O2_S2
 NAOH                      NAOH_S2                   NA2FEO2

Reject phase(s) /NONE/: HCP_A3
 HCP_A3  REJECTED
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

 .........................................................

    The following phases are retained in this system:

 AQUEOUS:A                 REF_ELECTRODE             GAS:G
 FCC_A1                    BCC_A2                    HALITE
 WUSTITE                   MAGNETITE                 HEMATITE
 FE2O3_GAMMA               FEO2H2                    FEO3H3
 FEOOH                     FE2O2O2H2                 NAO2
 NA2O                      NA2O_S2                   NA2O_S3
 NA2O2                     NA2O2_S2                  NAOH
 NAOH_S2                   NA2FEO2
```

```
 .......................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
      -Cl system.'
  'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
      -Cr-Na-Ni-C-H-O-N-S-Cl system.'
  'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
      -Na-Ni-C-H-O-N-S-Cl system.'
  'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
      only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
      from TCAQ2 which covers totally 83 elements and contains many more
      aqueous solution species.'
 -OK-
Should any phase have a miscibility gap check? /N/: N

      ...... Reinitializing POLY3 workspaces ......

Enforce Global Minimization Technique in calculations? /N/: N

Save all functions, variables and tables in POLY3 file? /Y/: Y

Set numerical limits? /N/: N


SET CALCULATING PARAMETERS:

 List of Default and Pre-defined Calculation Conditions:
 ---------------------------------------------------------------
  Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole
 ---------------------------------------------------------------
 T=298.15, P=1E5, B(H2O)=1000, N(H+1)=0, N(ZE)=0, N(CL)=0.1, N(FE)=1E-3,
    N(NA)=0.1
 DEGREES OF FREEDOM 0

Confirm defined conditions? /Y/: Y

 Calculating start points; please be patient!


LIST THE FIRST DEFAULT STARTING EQUILIBRIUM POINT:

 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 T=298.15, P=1E5, B(H2O)=1000, N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.1181, MUR(ZE)=100
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.57094E+01,  Mass in grams  1.00590E+03
 Total Gibbs energy -1.70696E+07,  Enthalpy -1.59069E+07,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 CL                      1.0000E-01  1.7950E-03 1.4499E-30 -1.7032E+05 SER
 FE                      1.0000E-03  1.7950E-05 4.6321E-26 -1.4461E+05 SER
 H+1                    -3.0000E-03 -5.3851E-05 1.0000E-07 -3.9956E+04 SER
 NA                      1.0000E-01  1.7950E-03 1.7205E-50 -2.8406E+05 SER
 H2O                     5.5508E+01  9.9639E-01 9.9593E-01 -1.0110E+01 AQUEOUS
 ZE                      3.0000E-03  5.3851E-05 1.0412E+00  1.0000E+02 REF_ELEC

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5707E+01, Mass 1.0058E+03, Volume fraction 0.0000E+00  Mole fractions:
 H2O  9.96410E-01  NA   1.79511E-03  FE   1.08146E-11
 CL   1.79511E-03  ZE   2.03381E-11  H+1 -1.36468E-11
 Constitution:           SiteFraction    Molality      Activity    log10Act
 H2O                      9.96410E-01   5.55084E+01   9.96012E-01    -0.0017
 CL-1                     1.79511E-03   1.00003E-01   7.76756E-02    -1.1097
 NA+1                     1.79511E-03   1.00003E-01   7.76756E-02    -1.1097
 OH-1                     2.31689E-09   1.29070E-07   1.00218E-07    -6.9991
 H+1                      2.30788E-09   1.28568E-07   1.00000E-07    -7.0000
 FE+2                     6.21477E-12   3.46215E-10   1.26203E-10    -9.8989
 FEOH+1                   4.59380E-12   2.55913E-10   1.99003E-10    -9.7011
 O3                       1.00000E-15   0.00000E+00   2.6033E-113  -112.5845
 H2O2                     1.00000E-15   0.00000E+00   3.63324E-46   -45.4397
 HCLO                     1.00000E-15   0.00000E+00   3.55905E-45   -44.4487
 H2                       1.00000E-15   0.00000E+00   5.46000E-18   -17.2628
 HCLO2                    1.00000E-15   0.00000E+00   1.38939E-87   -86.8572
 FEOH+2                   1.00000E-15   0.00000E+00   9.27035E-19   -18.0329
 HO2-1                    1.00000E-15   0.00000E+00   7.68880E-51   -50.1141
 FEO3H3-1                 1.00000E-15   0.00000E+00   1.69673E-51   -50.7704
 FECL+2                   1.00000E-15   0.00000E+00   3.39801E-23   -22.4688
 FE2O2H2+4                1.00000E-15   0.00000E+00   3.71405E-35   -34.4302
 FE+3                     1.00000E-15   0.00000E+00   1.53892E-23   -22.8128
 O2                       1.00000E-15   0.00000E+00   2.54948E-58   -57.5935
 CLO4-1                   1.00000E-15   0.00000E+00   8.8489E-133  -132.0531
 CLO3-1                   1.00000E-15   0.00000E+00   1.5694E-105  -104.8043
 CLO2-1                   1.00000E-15   0.00000E+00   1.45414E-82   -81.8374
 CLO2                     1.00000E-15   0.00000E+00   1.6417E-100   -99.7847
 CLO-1                    1.00000E-15   0.00000E+00   7.71560E-46   -45.1126
 CL2                      1.00000E-15   0.00000E+00   5.82418E-50   -49.2348
 Solution Properties:    pH =    7.0000    Eh =    0.0010 V     I =    0.1000
                         pe =    0.0175    Ah =    0.1000 kJ   m* =    0.2000
                         Aw =    0.9960    Os =    1.1089     pKw =  13.9973
                         At1= 1.0000E-15  At2= 1.2907E-07 (equiv_mol/kg_H2O)

 HEMATITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 2.5000E-03, Mass 7.9846E-02, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.20000E+00  FE   4.00000E-01  NA   0.00000E+00
 H2O  6.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00
 Constitution:
```

```
 FE2O3  1.00000E+00

LIST THE DEFINED SYMBOLS:
 DEFINED CONSTANTS
    TSLIMIT0=99, AH2O=55.508435, WH2O=1.80152E-2, RNL=2.3025851, R=8.31451,
       RNF=96485.309
 DEFINED FUNCTIONS AND VARIABLES%
    TC%=T-273.15
    PBAR%=P*1E-05
    PKB%=P*1E-08
    RT%=R*T
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
    YH2O=Y(AQUEOUS,H2O)
    ACRH2O=ACR(H2O,AQUEOUS)
    RCH2O=ACR(H2O,AQUEOUS)
    MLH2O=AH2O
    ACTW=ACRH2O
    OSMC=-YH2O/ (1-YH2O )* LOG(ACRH2O )
    TMI= (1-YH2O )*AH2O/YH2O
    AHZE=MUR(ZE)/1000
    PEZE=MUR(ZE)/ (RNL*RT )
    AI1=ACR(CL-1,AQUEOUS)*AH2O
    RC1=ACR(CL-1,AQUEOUS)*YH2O/Y(AQUEOUS,CL-1)
    ML1=Y(AQUEOUS,CL-1)*AH2O/YH2O
    AI2=ACR(CL2,AQUEOUS)*AH2O
    RC2=ACR(CL2,AQUEOUS)*YH2O/Y(AQUEOUS,CL2)
    ML2=Y(AQUEOUS,CL2)*AH2O/YH2O
    AI3=ACR(CLO-1,AQUEOUS)*AH2O
    RC3=ACR(CLO-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO-1)
    ML3=Y(AQUEOUS,CLO-1)*AH2O/YH2O
    AI4=ACR(CLO2,AQUEOUS)*AH2O
    RC4=ACR(CLO2,AQUEOUS)*YH2O/Y(AQUEOUS,CLO2)
    ML4=Y(AQUEOUS,CLO2)*AH2O/YH2O
    AI5=ACR(CLO2-1,AQUEOUS)*AH2O
    RC5=ACR(CLO2-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO2-1)
    ML5=Y(AQUEOUS,CLO2-1)*AH2O/YH2O
    AI6=ACR(CLO3-1,AQUEOUS)*AH2O
    RC6=ACR(CLO3-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO3-1)
    ML6=Y(AQUEOUS,CLO3-1)*AH2O/YH2O
    AI7=ACR(CLO4-1,AQUEOUS)*AH2O
    RC7=ACR(CLO4-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO4-1)
    ML7=Y(AQUEOUS,CLO4-1)*AH2O/YH2O
    AI8=ACR(FE+2,AQUEOUS)*AH2O
    RC8=ACR(FE+2,AQUEOUS)*YH2O/Y(AQUEOUS,FE+2)
    ML8=Y(AQUEOUS,FE+2)*AH2O/YH2O
    AI9=ACR(FE+3,AQUEOUS)*AH2O
    RC9=ACR(FE+3,AQUEOUS)*YH2O/Y(AQUEOUS,FE+3)
    ML9=Y(AQUEOUS,FE+3)*AH2O/YH2O
    AI10=ACR(FE2O2H2+4,AQUEOUS)*AH2O
    RC10=ACR(FE2O2H2+4,AQUEOUS)*YH2O/Y(AQUEOUS,FE2O2H2+4)
    ML10=Y(AQUEOUS,FE2O2H2+4)*AH2O/YH2O
    AI11=ACR(FECL+2,AQUEOUS)*AH2O
    RC11=ACR(FECL+2,AQUEOUS)*YH2O/Y(AQUEOUS,FECL+2)
    ML11=Y(AQUEOUS,FECL+2)*AH2O/YH2O
    AI12=ACR(FEO3H3-1,AQUEOUS)*AH2O
    RC12=ACR(FEO3H3-1,AQUEOUS)*YH2O/Y(AQUEOUS,FEO3H3-1)
    ML12=Y(AQUEOUS,FEO3H3-1)*AH2O/YH2O
    AI13=ACR(FEOH+1,AQUEOUS)*AH2O
    RC13=ACR(FEOH+1,AQUEOUS)*YH2O/Y(AQUEOUS,FEOH+1)
    ML13=Y(AQUEOUS,FEOH+1)*AH2O/YH2O
    AI14=ACR(FEOH+2,AQUEOUS)*AH2O
    RC14=ACR(FEOH+2,AQUEOUS)*YH2O/Y(AQUEOUS,FEOH+2)
    ML14=Y(AQUEOUS,FEOH+2)*AH2O/YH2O
    AI15=ACR(H+1,AQUEOUS)*AH2O
    RC15=ACR(H+1,AQUEOUS)*YH2O/Y(AQUEOUS,H+1)
    ML15=Y(AQUEOUS,H+1)*AH2O/YH2O
    AI16=ACR(H2,AQUEOUS)*AH2O
    RC16=ACR(H2,AQUEOUS)*YH2O/Y(AQUEOUS,H2)
    ML16=Y(AQUEOUS,H2)*AH2O/YH2O
    AI17=ACR(H2O,AQUEOUS)
    RC17=ACR(H2O,AQUEOUS)/Y(AQUEOUS,H2O)
    ML17=Y(AQUEOUS,H2O)*AH2O/YH2O
    AI18=ACR(H2O2,AQUEOUS)*AH2O
    RC18=ACR(H2O2,AQUEOUS)*YH2O/Y(AQUEOUS,H2O2)
    ML18=Y(AQUEOUS,H2O2)*AH2O/YH2O
    AI19=ACR(HCLO,AQUEOUS)*AH2O
    RC19=ACR(HCLO,AQUEOUS)*YH2O/Y(AQUEOUS,HCLO)
    ML19=Y(AQUEOUS,HCLO)*AH2O/YH2O
    AI20=ACR(HCLO2,AQUEOUS)*AH2O
    RC20=ACR(HCLO2,AQUEOUS)*YH2O/Y(AQUEOUS,HCLO2)
    ML20=Y(AQUEOUS,HCLO2)*AH2O/YH2O
    AI21=ACR(HO2-1,AQUEOUS)*AH2O
    RC21=ACR(HO2-1,AQUEOUS)*YH2O/Y(AQUEOUS,HO2-1)
    ML21=Y(AQUEOUS,HO2-1)*AH2O/YH2O
    AI22=ACR(NA+1,AQUEOUS)*AH2O
    RC22=ACR(NA+1,AQUEOUS)*YH2O/Y(AQUEOUS,NA+1)
    ML22=Y(AQUEOUS,NA+1)*AH2O/YH2O
    AI23=ACR(O2,AQUEOUS)*AH2O
    RC23=ACR(O2,AQUEOUS)*YH2O/Y(AQUEOUS,O2)
    ML23=Y(AQUEOUS,O2)*AH2O/YH2O
    AI24=ACR(O3,AQUEOUS)*AH2O
    RC24=ACR(O3,AQUEOUS)*YH2O/Y(AQUEOUS,O3)
    ML24=Y(AQUEOUS,O3)*AH2O/YH2O
    AI25=ACR(OH-1,AQUEOUS)*AH2O
    RC25=ACR(OH-1,AQUEOUS)*YH2O/Y(AQUEOUS,OH-1)
    ML25=Y(AQUEOUS,OH-1)*AH2O/YH2O
    IS1=.5*ML1+.5*ML3+.5*ML5
    IS2=.5*ML6+.5*ML7+.5*ML8*2**2
    IS3=.5*ML9*3**2+.5*ML10*4**2+.5*ML11*2**2
    IS4=.5*ML12+.5*ML13+.5*ML14*2**2
    IS5=.5*ML15+.5*ML21+.5*ML22
    ISTR=1*IS1+1*IS2+1*IS3+1*IS4+1*IS5
    RLOGH= LOG10(ACR(H+1,AQUEOUS)*AH2O )
    RLOGOH= LOG10(ACR(OH-1,AQUEOUS)*AH2O )
    RLOGH2O= LOG10(ACRH2O )
 DEFINED TABLES
    GPT=T, P, PH, EH, ISTR
    SFT=Y(AQUEOUS,CL-1), Y(AQUEOUS,CL2), Y(AQUEOUS,CLO-1), Y(AQUEOUS,CLO2),
       Y(AQUEOUS,CLO2-1), Y(AQUEOUS,CLO3-1), Y(AQUEOUS,CLO4-1),
       Y(AQUEOUS,FE+2), Y(AQUEOUS,FE+3), Y(AQUEOUS,FE2O2H2+4),
       Y(AQUEOUS,FECL+2), Y(AQUEOUS,FEO3H3-1), Y(AQUEOUS,FEOH+1),
       Y(AQUEOUS,FEOH+2), Y(AQUEOUS,H+1), Y(AQUEOUS,H2), Y(AQUEOUS,H2O),
       Y(AQUEOUS,H2O2), Y(AQUEOUS,HCLO), Y(AQUEOUS,HCLO2), Y(AQUEOUS,HO2-1),
       Y(AQUEOUS,NA+1), Y(AQUEOUS,O2), Y(AQUEOUS,O3), Y(AQUEOUS,OH-1), PH, EH
    AYT=AC(CL-1,AQUEOUS), AC(CL2,AQUEOUS), AC(CLO-1,AQUEOUS),
```

```
       AC(CLO2,AQUEOUS), AC(CLO2-1,AQUEOUS), AC(CLO3-1,AQUEOUS),
       AC(CLO4-1,AQUEOUS), AC(FE+2,AQUEOUS), AC(FE+3,AQUEOUS),
       AC(FE2O2H2+4,AQUEOUS), AC(FECL+2,AQUEOUS), AC(FEO3H3-1,AQUEOUS),
       AC(FEOH+1,AQUEOUS), AC(FEOH+2,AQUEOUS), AC(H+1,AQUEOUS),
       AC(H2,AQUEOUS), AC(H2O,AQUEOUS), AC(H2O2,AQUEOUS), AC(HCLO,AQUEOUS),
       AC(HCLO2,AQUEOUS), AC(HO2-1,AQUEOUS), AC(NA+1,AQUEOUS), AC(O2,AQUEOUS),
       AC(O3,AQUEOUS), AC(OH-1,AQUEOUS), PH, EH
    ART=ACR(CL-1,AQUEOUS), ACR(CL2,AQUEOUS), ACR(CLO-1,AQUEOUS),
       ACR(CLO2,AQUEOUS), ACR(CLO2-1,AQUEOUS), ACR(CLO3-1,AQUEOUS),
       ACR(CLO4-1,AQUEOUS), ACR(FE+2,AQUEOUS), ACR(FE+3,AQUEOUS),
       ACR(FE2O2H2+4,AQUEOUS), ACR(FECL+2,AQUEOUS), ACR(FEO3H3-1,AQUEOUS),
       ACR(FEOH+1,AQUEOUS), ACR(FEOH+2,AQUEOUS), ACR(H+1,AQUEOUS),
       ACR(H2,AQUEOUS), ACR(H2O,AQUEOUS), ACR(H2O2,AQUEOUS),
       ACR(HCLO,AQUEOUS), ACR(HCLO2,AQUEOUS), ACR(HO2-1,AQUEOUS),
       ACR(NA+1,AQUEOUS), ACR(O2,AQUEOUS), ACR(O3,AQUEOUS), ACR(OH-1,AQUEOUS),
       PH, EH
    AIT=AI1, AI2, AI3, AI4, AI5, AI6, AI7, AI8, AI9, AI10, AI11, AI12, AI13,
       AI14, AI15, AI16, AI17, AI18, AI19, AI20, AI21, AI22, AI23, AI24, AI25,
       PH, EH
    RCT=RC1, RC2, RC3, RC4, RC5, RC6, RC7, RC8, RC9, RC10, RC11, RC12, RC13,
       RC14, RC15, RC16, RC17, RC18, RC19, RC20, RC21, RC22, RC23, RC24, RC25,
       PH, EH
    MLT=ML1, ML2, ML3, ML4, ML5, ML6, ML7, ML8, ML9, ML10, ML11, ML12, ML13,
       ML14, ML15, ML16, ML18, ML19, ML20, ML21, ML22, ML23, ML24, ML25, ISTR,
       PH, EH

 IMPORTANT FACTS:
     The default definitions of the Eh and pH quantities in the
       advanced POURBAIX-Module (and in the ordinary TDB-GES-POLY
       calculation routines) should ALWAYS be as below:
         Eh = MUR(ZE)/RNF
         pH = -log10[AI(H+1,AQUEOUS)]
            = -log10[ACR(H+1,AQUEOUS)*AH2O]
       where RNF is the Faraday constant (96485.309 C/mol),
       and AH2O is the molecular weight of H2O (55.508435 g).
       MUR(ZE) is the electrochemical potential (ECP; in the
       unit of J/mol; w.r.t. the standard hydrogen electrode).
       ACR(H+1,AQUEOUS) is the site-fraction-based activity of
       the H+1 aqueous species in AQUEOUS solution phase, but
       AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH2O] is
       the molality-based activity of the H+1 aqueous species
       that should be used for defining the pH quantity.

     Within an aqueous-bearing heterogeneous interaction system,
       the fundamental system-components must be H2O, H+1 and ZE,
       which are corresponding to the basic elements O & H and
       the hypothetical electron (ZE) in the aqueous solution
       phase. For the additional chemical elements in the system,
       their corresponding system-components shall be defined as
       in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S)
       or (for some) in their molecular forms (e.g., NaCl, H2S).
       The reference state for the H2O component must always be
       defined as the solvent species H2O in the AQUEOUS solution
       phase under the current temperature (*) and 100000 Pascal
       (i.e., 1 bar). The reference states for the H+1 and ZE
       components are by default set as their SER.

     Various conventional properties of aqueous solute species I
       are converted in the following manners:
         ML = Y(AQUEOUS,I)*AH2O/YH2O
         RC = ACR(I,AQUEOUS)*YH2O/Y(AQUEOUS,I)
         AI = RC*ML
            = ACR(I,AQUEOUS)*AH2O
       where YH2O [i.e., Y(AQUEOUS,H2O)] and Y(AQUEOUS,I) are
       the site-fractions of solvent H2O and solute species I.

LIST THE DEFINED AXIS-VARIABLES:

  Axis No 1: LNACR(H+1)            Min: -34.532608Max: 2.3025851 Inc: 0.8
  Axis No 2: MUR(ZE)               Min: -150000   Max: 200000    Inc: 7718.85

     NOTE: The default settings (listed above) for two mapping
           variables [in terms of lnACR(H+1) and MUR(ZE), and
           their minimum/maximum values and increment steps]
           are covering the following pH-Eh ranges/steps:
             pH:  0.00 -> 14.00, at a step of 0.35
             Eh: -1.55 ->  2.07, at a step of 0.08 (V)

           The maximum pH limit has been calculated precisely
           and determined automatically by the POURBAIX-Module,
           as a function of the temperature-pressure conditions
           and initial bulk compositions of the current defined
           interaction system.

Accept the default settings for two mapping variables? /Y/: Y


LIST ALL THE INITIAL EQUILIBRIA FOR MAPPING:

 No 1  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 2  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 3  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 4  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 5  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=-28400
 No 6  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=-28400
 No 7  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=-28400
 No 8  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=-28400
 No 9  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
 No 10 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
 No 11 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
 No 12 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
 No 13 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 14 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
```

```
    LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 15 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 16 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 17 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=66000.
 No 18 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=66000.
 No 19 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=66000.
 No 20 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=66000.


 MAP THE POURBAIX DIAGRAM:
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
 Generating start point  31
 Generating start point  32
 Generating start point  33
 Generating start point  34
 Generating start point  35
 Generating start point  36
 Generating start point  37
 Generating start point  38
 Generating start point  39
 Generating start point  40
 Working hard
 Generating start point  41
 Generating start point  42
 Generating start point  43
 Generating start point  44
 Generating start point  45
 Generating start point  46

 Phase region boundary   1 at:  -1.612E+01  7.911E+04
     GAS
     AQUEOUS
  ** HALITE
     HEMATITE
 Calculated..                     25  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:  -3.453E+01  3.383E+04
     GAS
     AQUEOUS
  ** HALITE
     HEMATITE
 Calculated.                     42  equilibria

 Phase region boundary   3 at:  -2.296E+00  1.134E+05
     GAS
     AQUEOUS
  ** HALITE
  ** HEMATITE

 Phase region boundary   4 at:  -2.296E+00  1.134E+05
     GAS
     AQUEOUS
  ** HALITE
 Calculated                     33  equilibria

 Phase region boundary   5 at:  -2.296E+00  1.134E+05
     GAS
     AQUEOUS
  ** HEMATITE
 Calculated                      5  equilibria

 Phase region boundary   6 at:  -2.296E+00  1.134E+05
     GAS
     AQUEOUS
     HALITE
  ** HEMATITE
 Calculated                     31  equilibria

 Phase region boundary   7 at:  -1.612E+01  7.911E+04
     GAS
```

```
    AQUEOUS
 ** HALITE
    HEMATITE
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary   8 at:  -1.612E+01  7.817E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     26  equilibria
Terminating at axis limit.

Phase region boundary   9 at:  -3.453E+01  3.296E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     43  equilibria

Phase region boundary  10 at:  -1.975E+00  1.132E+05
 ** GAS
    AQUEOUS
 ** HEMATITE

Phase region boundary  11 at:  -1.975E+00  1.132E+05
 ** GAS
    AQUEOUS
Calculated..                      9  equilibria
Terminating at axis limit.

Phase region boundary  12 at:  -1.975E+00  1.132E+05
    AQUEOUS
 ** HEMATITE
Calculated.                     30  equilibria

Phase region boundary  13 at:  -1.420E+01 -2.225E+04
    AQUEOUS
 ** HEMATITE
 ** MAGNETITE

Phase region boundary  14 at:  -1.420E+01 -2.225E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated..                     30  equilibria
Terminating at axis limit.

Phase region boundary  15 at:  -1.420E+01 -2.225E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                      4  equilibria

Phase region boundary  16 at:  -1.625E+01 -4.067E+04
 ** GAS
    AQUEOUS
 ** MAGNETITE

Phase region boundary  17 at:  -1.625E+01 -4.067E+04
    GAS
    AQUEOUS
 ** MAGNETITE
Calculated                     34  equilibria

Phase region boundary  18 at:  -1.625E+01 -4.067E+04
 ** GAS
    AQUEOUS
Calculated..                     28  equilibria
Terminating at axis limit.

Phase region boundary  19 at:  -1.625E+01 -4.067E+04
 ** GAS
    AQUEOUS
    MAGNETITE
Calculated..                     27  equilibria
Terminating at axis limit.

Phase region boundary  20 at:  -1.420E+01 -2.225E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
Calculated..                     30  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  21 at:  -1.975E+00  1.132E+05
    GAS
    AQUEOUS
 ** HEMATITE
Calculated                     11  equilibria

Phase region boundary  22 at:  -1.612E+01  7.817E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:  -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
Calculated..                     26  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:  -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:  -1.116E+01  1.000E+02
    AQUEOUS
 ** HEMATITE
Calculated.                      7  equilibria
```

```
Terminating at known equilibrium

Phase region boundary  26 at:  -1.116E+01  1.000E+02
    AQUEOUS
 ** HEMATITE
Calculated.                     24  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:  -1.612E+01 -2.701E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated..                     26  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:  -1.612E+01 -2.701E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  29 at:  -1.612E+01 -3.959E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:  -1.612E+01 -3.959E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:  -1.485E+01 -2.840E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:  -1.485E+01 -2.840E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  33 at:  -1.668E+01 -2.840E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated..                     26  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  34 at:  -1.668E+01 -2.840E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated.                      5  equilibria
Terminating at known equilibrium

Phase region boundary  35 at:  -9.172E+00  9.539E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     35  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  36 at:  -9.172E+00  9.539E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:  -9.210E+00  9.529E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     35  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  38 at:  -9.210E+00  9.529E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:  -9.210E+00  1.461E+04
    AQUEOUS
 ** HEMATITE
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:  -9.210E+00  1.461E+04
    AQUEOUS
 ** HEMATITE
Calculated.                     25  equilibria
Terminating at known equilibrium

Phase region boundary  41 at:  -9.210E+00 -2.323E+04
 ** GAS
    AQUEOUS
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  42 at:  -9.210E+00 -2.323E+04
 ** GAS
    AQUEOUS
Calculated..                     18  equilibria
Terminating at known equilibrium
Terminating at axis limit.
```

```
Phase region boundary  43 at:  -5.086E+00 -1.300E+04
 ** GAS
    AQUEOUS
Calculated.                     16  equilibria
Terminating at known equilibrium

Phase region boundary  44 at:  -5.086E+00 -1.300E+04
 ** GAS
    AQUEOUS
Calculated..                     13  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  45 at:  -1.293E+01 -1.300E+04
    AQUEOUS
 ** HEMATITE
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  46 at:  -1.293E+01 -1.300E+04
    AQUEOUS
 ** HEMATITE
Calculated.                     27  equilibria
Terminating at known equilibrium

Phase region boundary  47 at:  -9.210E+00  9.529E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     35  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  48 at:  -9.210E+00  9.529E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  49 at:  -9.210E+00 -2.323E+04
 ** GAS
    AQUEOUS
Calculated.                     10  equilibria
Terminating at known equilibrium

Phase region boundary  50 at:  -9.210E+00 -2.323E+04
 ** GAS
    AQUEOUS
Calculated..                     18  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  51 at:  -9.210E+00  1.461E+04
    AQUEOUS
 ** HEMATITE
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  52 at:  -9.210E+00  1.461E+04
    AQUEOUS
 ** HEMATITE
Calculated.                     25  equilibria
Terminating at known equilibrium

Phase region boundary  53 at:  -1.975E+00  8.684E+04
    AQUEOUS
 ** HEMATITE
Calculated.                     26  equilibria
Terminating at known equilibrium

Phase region boundary  54 at:  -1.975E+00  8.684E+04
    AQUEOUS
 ** HEMATITE
Calculated.                      5  equilibria
Terminating at known equilibrium

Phase region boundary  55 at:  -1.262E+01  8.684E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     31  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  56 at:  -1.262E+01  8.684E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  57 at:  -1.612E+01  7.817E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     26  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  58 at:  -1.612E+01  7.817E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary  59 at:  -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
Calculated..                     26  equilibria
Terminating at known equilibrium
Terminating at axis limit.
```

```
 Phase region boundary  60 at:  -1.612E+01 -2.701E+04
     AQUEOUS
     HEMATITE
  ** MAGNETITE
 Calculated.                        4  equilibria
 Terminating at known equilibrium

 Phase region boundary  61 at:  -2.438E+00  6.600E+04
     AQUEOUS
  ** HEMATITE
 Calculated.                       24  equilibria
 Terminating at known equilibrium

 Phase region boundary  62 at:  -2.438E+00  6.600E+04
     AQUEOUS
  ** HEMATITE
 Calculated.                        9  equilibria
 Terminating at known equilibrium

 Phase region boundary  63 at:  -2.103E+01  6.600E+04
  ** GAS
     AQUEOUS
     HEMATITE
 Calculated..                       20  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

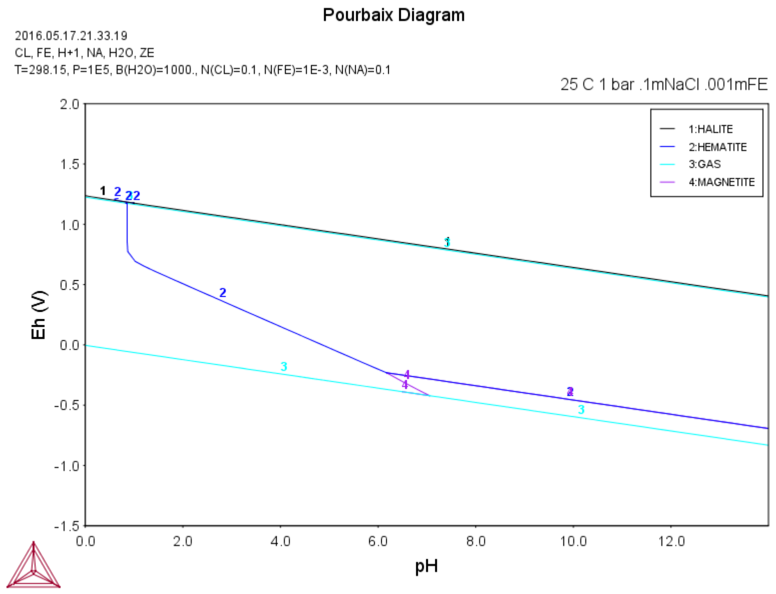
 Phase region boundary  64 at:  -2.103E+01  6.600E+04
  ** GAS
     AQUEOUS
     HEMATITE
 Calculated.                       26  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex40\POUR
 BAIX.POLY3
 CPU time for mapping                    225  seconds

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

 CURRENT DEVICE: TC-UNITE Driver

 Plotting the diagram; please be patient!
```



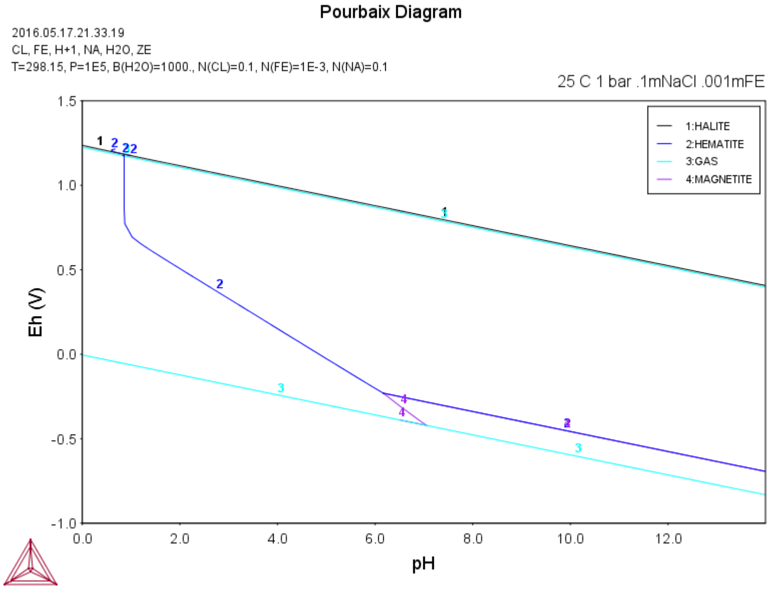
```
Hit RETURN to continue

Any missing phase boundary you could possibly think of? /N/:  ?
 ---------------------------------------------------------------
 Sometimes the POURBAIX Module may miss some phase boundaries
   due to various reasons during the mapping process.
 By answering "Yes" here, the user would be able to add some
   additional starting point(s) into the calculation. In the
   following steps, the user will be asked to specify a pH-Eh
   coordinate pair, for instance (4.0, -0.15), which is close
   to the expected phase boundary.
 However, such additional pH-Eh point should not outside the
   AQUEOUS/GAS(O2) or AQUEOUS/GAS(H2) boundaries; otherwise,
   the module will fail in finding any new starting point.

Any missing phase boundary you could possibly think of? /N/: N

Change the pH/Eh steps for smoother curves? /N/: N

Zoom in? /N/: y
 Change scaling of X-axis? /N/:  N
 Change scaling of Y-axis? /N/:  y
  Minimum /-1.2/:    -1.0
  Maximum /1.5/:     1.5
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
 CURRENT DEVICE: TC-UNITE Driver
 Plotting the diagram; please be patient!
```



```
Hit RETURN to continue

Another zoom? /N/:  N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: n

Save X-Y coordinates of curve on text file? /N/: y
File name /POURBAIX/:   TCEX40-1.EXP

Modify the diagram? /N/: y

Zoom in? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: y

 At what pH-Eh point add the label text?
      X-pH /1.2/:   1.2
      Y-Eh /.25/:   0.25
  Automatic phase labels? /N/:   N
      Text? /Aqs/:   Aqs
Text size: /.36/:   0.26

Another Label Text to be added? /N/:  y

 At what pH-Eh point add the label text?
      X-pH /2.599732093/:   8
      Y-Eh /.5/:   0.25
  Automatic phase labels? /N/:   N
      Text? /Aqs/:   Aqs+Hm
Text size: /.36/:   0.26

Another Label Text to be added? /N/:  y

 At what pH-Eh point add the label text?
      X-pH /9.399732093/:   8
      Y-Eh /.5/:   -0.3
  Automatic phase labels? /N/:   N
      Text? /Aqs/:   Aqs+Mt
Text size: /.36/:   0.26

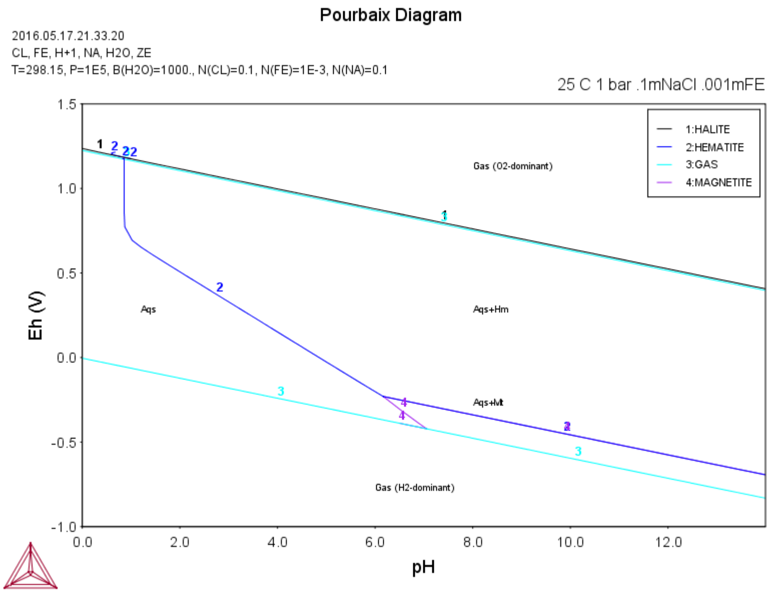
Another Label Text to be added? /N/:  y

 At what pH-Eh point add the label text?
      X-pH /9.399732093/:   8
      Y-Eh /-.05/:   1.1
  Automatic phase labels? /N/:   N
      Text? /Aqs/:   Gas (O2-dominant)
Text size: /.36/:   0.26

Another Label Text to be added? /N/:  y

 At what pH-Eh point add the label text?
      X-pH /9.399732093/:   6
      Y-Eh /1.35/:   -.8
  Automatic phase labels? /N/:   N
      Text? /Aqs/:   Gas (H2-dominant)
Text size: /.36/:   .26

Another Label Text to be added? /N/:  N
```

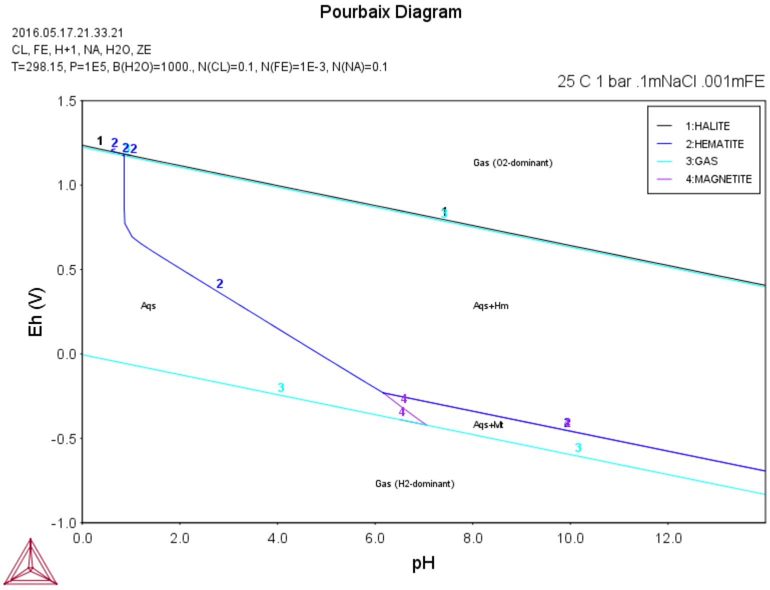


```
Hit RETURN to continue

Modify Label-Texts on the Pourbaix diagram? /N/: y
 These labels are defined
 No    1 at  1.20000E+00 2.50000E-01 : Aqs
 No    2 at  8.00000E+00 2.50000E-01 : Aqs+Hm
 No    3 at  8.00000E+00-3.00000E-01 : Aqs+Mt
 No    4 at  8.00000E+00 1.10000E+00 : Gas (O2-dominant)
 No    5 at  6.00000E+00-8.00000E-01 : Gas (H2-dominant)

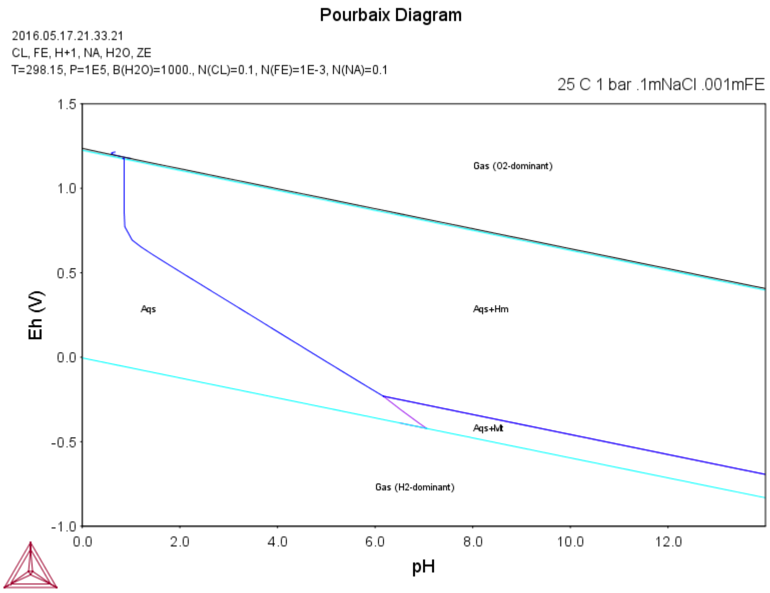
Which label to modify? /5/:  3
New X coordinate /8/:   8
New Y coordinate /-.3/:   -.45
New text /Aqs+Mt/:   Aqs+Mt

Another Label Text to be modified? /N/:  N
```



```
Hit RETURN to continue

Modify Label-Curve-Option on the Pourbaix diagram? /N/: y
Curve-Label Option? /E/:  ?
 THE OPTIONS MEANS:
 A      LIST STABLE PHASES ALONG LINE
 B      AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
 C      LIST AXIS QUANTITIES
 D      AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
 E      AS B WITH CHANGING COLORS
 F      AS D WITH CHANGING COLORS
 N      NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /E/:  n
```



```
Hit RETURN to continue

Another Curve-Label Option? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: N

Modify Label-Texts on the Pourbaix diagram? /N/: N

Modify Label-Curve-Option on the Pourbaix diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: y

Zoom in? /N/:  N

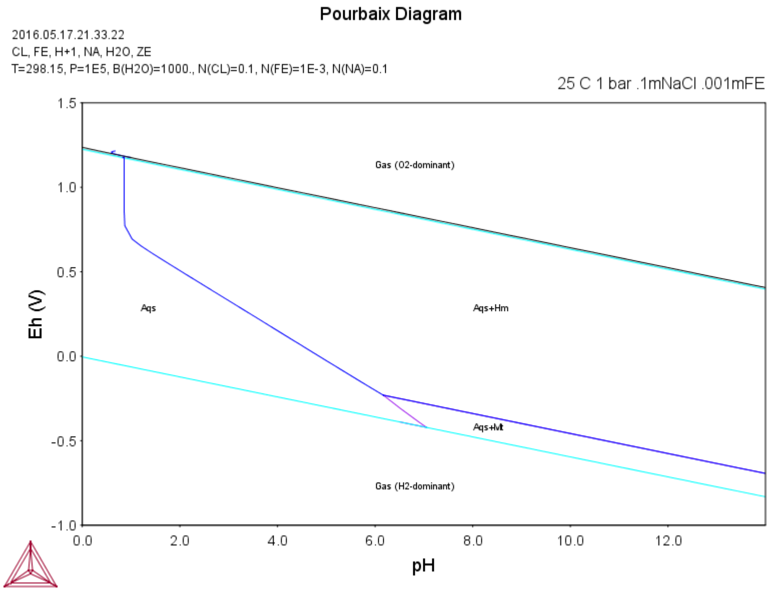
Change Curve-Label Option for the diagram? /N/:  N

Add Label-Texts onto the Pourbaix diagram? /N/:  N

Modify Label-Texts on the Pourbaix diagram? /N/:  y
 These labels are defined
 No   1 at  1.20000E+00 2.50000E-01 : Aqs
 No   2 at  8.00000E+00 2.50000E-01 : Aqs+Hm
 No   3 at  8.00000E+00-4.50000E-01 : Aqs+Mt
 No   4 at  8.00000E+00 1.10000E+00 : Gas (O2-dominant)
 No   5 at  6.00000E+00-8.00000E-01 : Gas (H2-dominant)

Which label to modify? /5/:   4
New X coordinate /8/:   6
New Y coordinate /1.1/:   1.1
New text /Gas (O2-dominant)/:   Gas (O2-dominant)

Another Label Text to be modified? /N/:  N
```



```
Hit RETURN to continue

Modify Label-Curve-Option on the Pourbaix diagram? /N/: N

Change the Subtitle of the diagram? /N/: N
```

```
Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: y

  Loading workspaces from the POLY3 file: POURBAIX

 The loaded POLY3 file is of POURBAIX-MAPPING Calculation.

 The current system consists of  6 elements:
    CL FE H  NA O  ZE

 List of Default and Pre-defined Calculation Conditions:
 --------------------------------------------------------------
  Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole
 --------------------------------------------------------------
 T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.1181, MUR(ZE)=66000.
 FIXED PHASES
 GAS=0
 DEGREES OF FREEDOM -1

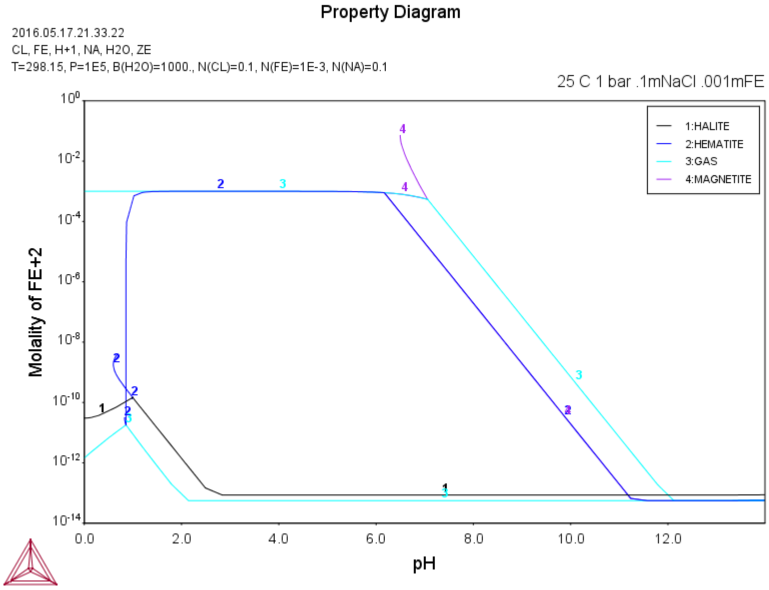
SET PLOTTING PARAMETERS:

   ------------------------------------------------------------
   I                                                          I
   I   The following properties are available to be selected I
   I     as axis variables for making other diagrams from the I
   I     same calculation:                                    I
   I                                                          I
   I          pH  --- Acidity                                 I
   I          Eh  --- Electronic Potential (V)                I
   I          Ah  --- Electronic Affinity  (kJ)               I
   I          pe  --- Electronic Activity (log10ACRe)         I
   I          IS  --- Ionic Strength                          I
   I          TM  --- Total Concentration                     I
   I          Aw  --- Activity of Water                       I
   I          Oc  --- Osmotic Coefficient                     I
   I     MF(AQsp) --- Mole Fractions of Aqueous Species       I
   I     ML(AQsp) --- Molalities of Aqueous Species           I
   I     AI(AQsp) --- Activities of Aqueous Species           I
   I     RC(AQsp) --- Activity Coefficients of Aq Species     I
   I                                                          I
   I  where "AQsp" is the name of a specific aqueous species, I
   I    and "*" can be used as a wild sign for all "AQsp";    I
   I  It is unnecessary to give a complete aqueous species    I
   I    names; however, the entered AQsp name must be unique. I
   I  If neither "AQsp" nor "*" is given here, all species    I
   I    will be searched.                                     I
   I                                                          I
   I__________________________________________________________I


   List of All the AQsp (Aqueous Species) in the Defined System:
   =================================================================
    CL-1         CL2          CLO-1        CLO2         CLO2-1
    CLO3-1       CLO4-1       FE+2         FE+3         FE2O2H2+4
    FECL+2       FEO3H3-1     FEOH+1       FEOH+2       H+1
    H2           H2O          H2O2         HCLO         HCLO2
    HO2-1        NA+1         O2           O3           OH-1

   -----------------------------------------------------------------

 X-axis Variable: /PH/:  pH
 Y-axis Variable: /EH/:  ml(fe+2)
 CURRENT DEVICE: TC-UNITE Driver
 Plotting the diagram; please be patient!
```

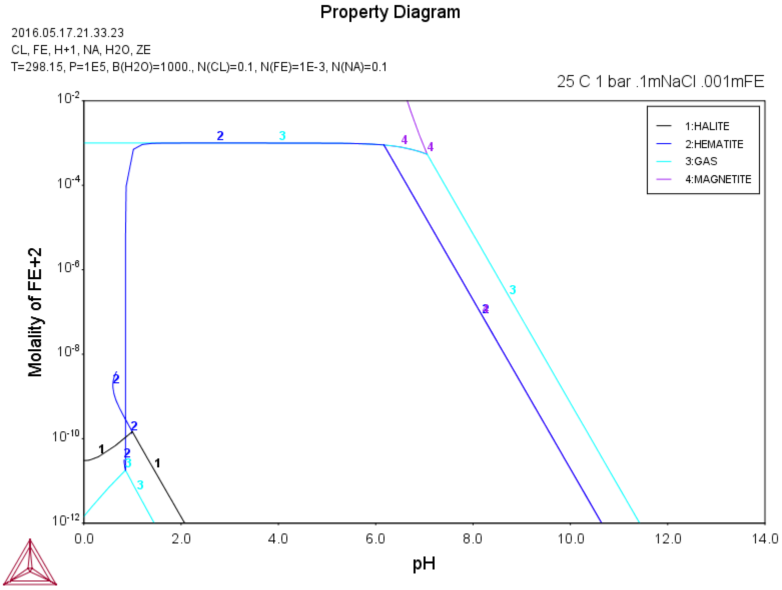


```
Hit RETURN to continue

Change axis type? /N/: N

Zoom in? /N/: y
 Change scaling of X-axis? /N/:  y
  Minimum /0/:     0
  Maximum /13.99557858/:   14
```

```
 Change scaling of Y-axis? /N/:  y
  Minimum /1E-40/:   1e-12
  Maximum /1/:   1e-2
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
 CURRENT DEVICE: TC-UNITE Driver
 Plotting the diagram; please be patient!
```



```
Hit RETURN to continue

Another zoom? /N/:  N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the specified diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: y


  Loading workspaces from the POLY3 file: POURBAIX

 The loaded POLY3 file is of POURBAIX-MAPPING Calculation.

 The current system consists of  6 elements:
    CL  FE  H   NA  O   ZE

 List of Default and Pre-defined Calculation Conditions:
 ---------------------------------------------------------------
  Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole
 ---------------------------------------------------------------
 T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.1181, MUR(ZE)=66000.
 FIXED PHASES
 GAS=0
 DEGREES OF FREEDOM -1

SET PLOTTING PARAMETERS:

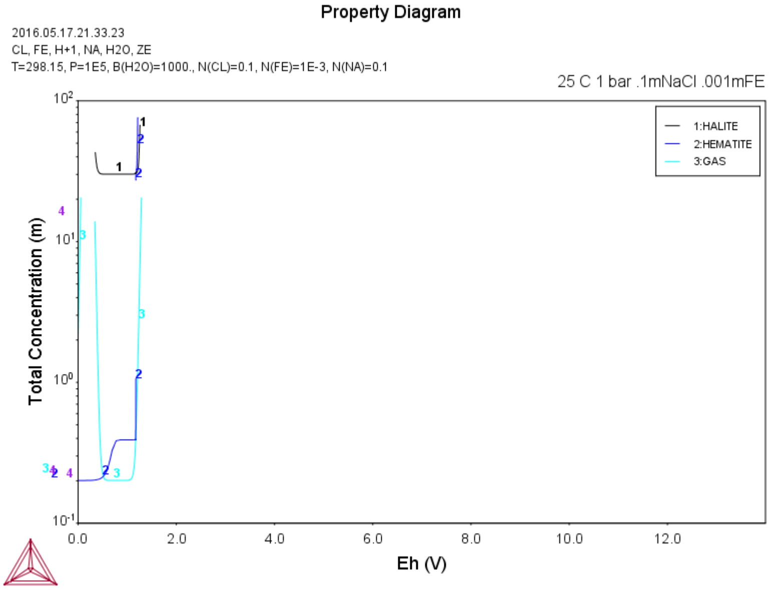
   ------------------------------------------------------------
   I                                                          I
   I   The following properties are available to be selected  I
   I     as axis variables for making other diagrams from the I
   I     same calculation:                                    I
   I                                                          I
   I          pH  --- Acidity                                 I
   I          Eh  --- Electronic Potential (V)                I
   I          Ah  --- Electronic Affinity  (kJ)               I
   I          pe  --- Electronic Activity (log10ACRe)         I
   I          IS  --- Ionic Strength                          I
   I          TM  --- Total Concentration                     I
   I          Aw  --- Activity of Water                       I
   I          Oc  --- Osmotic Coefficient                     I
   I     MF(AQsp) --- Mole Fractions of Aqueous Species       I
   I     ML(AQsp) --- Molalities of Aqueous Species           I
   I     AI(AQsp) --- Activities of Aqueous Species           I
   I     RC(AQsp) --- Activity Coefficients of Aq Species     I
   I                                                          I
   I  where "AQsp" is the name of a specific aqueous species, I
   I    and "*" can be used as a wild sign for all "AQsp";    I
   I  It is unnecessary to give a complete aqueous species    I
   I    names; however, the entered AQsp name must be unique. I
   I  If neither "AQsp" nor "*" is given here, all species    I
   I    will be searched.                                     I
   I                                                          I
   I__________________________________________________________I


   List of All the AQsp (Aqueous Species) in the Defined System:
   ================================================================
    CL-1         CL2          CLO-1        CLO2         CLO2-1
    CLO3-1       CLO4-1       FE+2         FE+3         FE2O2H2+4
```

```
    FECL+2       FEO3H3-1     FEOH+1       FEOH+2       H+1
    H2           H2O          H2O2         HCLO         HCLO2
    HO2-1        NA+1         O2           O3           OH-1

   ----------------------------------------------------------------

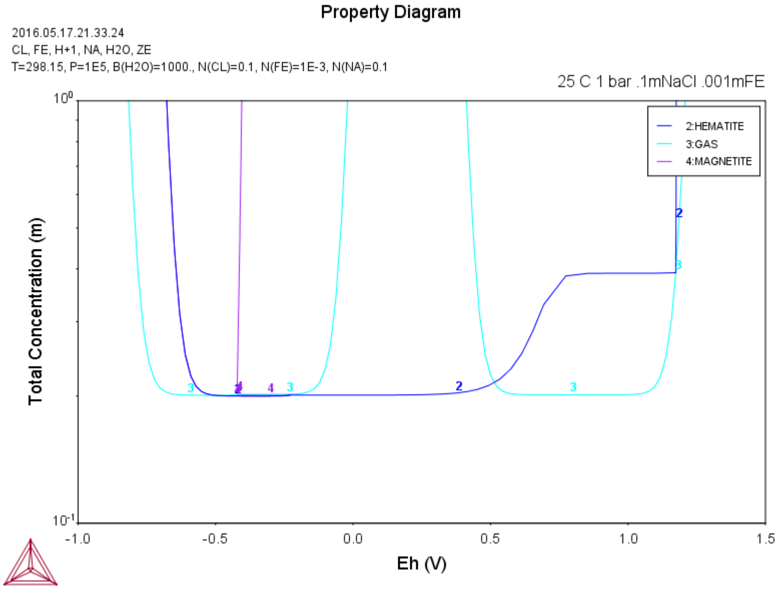
 X-axis Variable: /PH/:  Eh
 Y-axis Variable: /ML/:  TM
 CURRENT DEVICE: TC-UNITE Driver
 Plotting the diagram; please be patient!
```



```
Hit RETURN to continue

Change axis type? /N/: N

Zoom in? /N/: y
 Change scaling of X-axis? /N/:  y
  Minimum /-1.2/:   -1.0
  Maximum /1.5/:    1.5
 Change scaling of Y-axis? /N/:  y
  Minimum /1E-08/:   0.1
  Maximum /100/:   1
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
 CURRENT DEVICE: TC-UNITE Driver
 Plotting the diagram; please be patient!
```



```
Hit RETURN to continue

Another zoom? /N/:  N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the specified diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: N

SYS:
```

```
SYS: @@... Up to this point, the POURBAIX-module run has accomplished!
SYS:
SYS: @@
SYS: @@ Under MS-Windows, one can optionally use the DOS-command "copy"
SYS: @@   to backup the resulted POURBAIX.POLY3 file as TCEX40.POLY3:
SYS: @@
SYS: @copy POURBAIX.POLY3 TCEX40.POLY3
        1 fil(er) kopierad(e).
SYS:
SYS: SET_INTERACTIVE
   ... the command in full is SET_INTERACTIVE_MODE
SYS:
```

tcex41

```
SYS:About
 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex41\tcex41.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of a solubility product
SYS: @@
SYS: set-log ex41,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .19
2nd alloying element: mn 1.16
Next alloying element: si .2
Next alloying element: cr .72
Next alloying element: ni .2
Next alloying element: mo .08
Next alloying element: cu .26
Next alloying element: al .027
Next alloying element: n .0089
Next alloying element:
Temperature (C) /1000/: 1056
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MO  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CU  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 AL  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 N  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M6C                      M5C2
 M3C2                     MC_ETA                   MC_SHP
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 Z_PHASE                  FE4N_LP1                 FECN_CHI
 PI                       SIGMA                    MU_PHASE
 P_PHASE                  R_PHASE                  CHI_A12
 LAVES_PHASE_C14          M3SI                     G_PHASE
 CR3SI                    FE2SI                    MSI
 M5SI3                    NBNI3                    NI3TI
 AL4C3                    FE8SI2C                  SIC
 ALN                      SI3N4                    MN6N4
 MN6N5

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

 ........................................................

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M6C                      M5C2
 M3C2                     MC_ETA                   MC_SHP
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 Z_PHASE                  FE4N_LP1                 FECN_CHI
 PI                       SIGMA                    MU_PHASE
 P_PHASE                  R_PHASE                  CHI_A12
 LAVES_PHASE_C14          M3SI                     G_PHASE
```

```
 CR3SI                     FE2SI                     MSI
 M5SI3                     NBNI3                     NI3TI
 AL4C3                     FE8SI2C                   SIC
 ALN                       SI3N4                     MN6N4
 MN6N5

 .........................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'S. Jonsson, Metall. Trans. A, 23A (1992), 3141-3149; Al-Fe-N'
  'J. Grobner, H.-L. Lukas and F. Aldinger, J. Alloys Compounds, 220 (1995),
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  'N. Subasic licentiate thesis 2000, KTH, Sweden'
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  'M. Seiersten, unpublished work (1989); Al-Fe'
  'A. Jansson, Metall. Trans. 23A (1992) 2953-2962; AL-MN'
  'N. Saunders, COST 507 Report (1998); Al-Mo'
  'I. Ansara, N. Dupin, H.-L. Lukas and B. Sundman, J. Alloys and Compounds,
       247 (1997), 20-30; Al-Ni'
  'T. Godecke, F. Sommer and H.-L. Lukas, unpublished work (1996); Al-Si
       parameters available from J. Grobner et al., Calphad, 20 (1996), 247;
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  'P. Gustafson, Inst. Met. Res. (IM-2549, 1990); C-CU-FE'
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       -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'J-O. Andersson, Calphad, 12 (1988), 1-8; TRITA 0317 (1986); C-MO'
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       and Al-Si-C'
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  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'B.-J. Lee, Metall. Trans. A, 24A (1993), 1919-1933; Cr-Mn, Fe-Cr-Mn'
  'K. Frisk, KTH Report D 60 (1984); CR-MO'
  'K. Frisk, TRITA-MAC 393 (1989); CR-N, FE-N, MO-N, CR-MO-N'
  'B.-J. Lee, KRISS, unpublished research, during 1993-1995'
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  'K. Frisk, IM-2929, Swedish Inst. Met. Res., (1992); Cu-N, Fe-Cu-N'
  'S. an Mey, Calphad 16 (1992) 255-260; Cu-Ni'
  'M. Jacobs (1991), Revised by T. Buehler (1997), COST 507 Report; Cu-Si'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'A. Fernandez Guillermet, Calphad, 6 (1982), 127-140; (sigma phase revised
       1986); TRITA-MAC 200 (1982); FE-MO'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;
       Fe-Si and Fe-Si-C'
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 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         29105 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     2  s
POLY_3:
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1329.15, W(C)=1.9E-3, W(MN)=1.16E-2, W(SI)=2E-3, W(CR)=7.2E-3, W(NI)=2E-3,
    W(MO)=8E-4, W(CU)=2.6E-3, W(AL)=2.7E-4, W(N)=8.9E-5, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1329.15 K (  1056.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53245E+01
 Total Gibbs energy -6.89251E+04,  Enthalpy  3.91376E+04,  Volume  7.33525E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      5.5361E-04  2.7000E-04 1.6468E-09 -2.2351E+05 SER
 C                       8.7517E-03  1.9000E-03 8.6247E-03 -5.2528E+04 SER
 CR                      7.6609E-03  7.2000E-03 7.6112E-05 -1.0480E+05 SER
 CU                      2.2636E-03  2.6000E-03 1.0015E-04 -1.0177E+05 SER
 FE                      9.6245E-01  9.7154E-01 2.2979E-03 -6.7145E+04 SER
 MN                      1.1682E-02  1.1600E-02 1.1078E-05 -1.2610E+05 SER
 MO                      4.6133E-04  8.0000E-04 9.9033E-06 -1.2734E+05 SER
 N                       3.5153E-04  8.9000E-05 5.1545E-07 -1.6000E+05 SER
 NI                      1.8853E-03  2.0000E-03 2.7230E-06 -1.4161E+05 SER
 SI                      3.9396E-03  2.0000E-03 5.2580E-09 -2.1068E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.9974E-01, Mass 5.5319E+01, Volume fraction 9.9977E-01  Mass fractions:
 FE  9.71636E-01  CU  2.60025E-03  C   1.90019E-03  N   5.57073E-05
 MN  1.16011E-02  SI  2.00019E-03  MO  8.00078E-04
```

```
 CR  7.20070E-03  NI  2.00019E-03  AL  2.05877E-04

 ALN                          Status ENTERED     Driving force  0.0000E+00
 Moles 2.6304E-04, Mass 5.3909E-03, Volume fraction 2.2895E-04  Mass fractions:
 AL  6.58274E-01  NI  0.00000E+00  FE  0.00000E+00  C   0.00000E+00
 N   3.41726E-01  MO  0.00000E+00  CU  0.00000E+00
 SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: def-dia
   ... the command in full is DEFINE_DIAGRAM
Same elements as before? /Y/: Y
 For binary or ternary diagrams you may prefer the special modules

 You must specify a value for all compositions and the temperature even
 if you want to use it as axis.
Mass (weight) percent of AL /.027/: .027
Mass (weight) percent of C /.19/: .19
Mass (weight) percent of CR /.72/: .72
Mass (weight) percent of CU /.26/: .26
Mass (weight) percent of MN /1.16/: 1.16
Mass (weight) percent of MO /.08/: .08
Mass (weight) percent of N /.0089/: .0089
Mass (weight) percent of NI /.2/: .2
Mass (weight) percent of SI /.2/: .2
Temperature (C) /1056/: 1056
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
 You must now set an independent axis for your diagram
 as one of the following conditions:
 Condition  1 is temperature (Celsius)
 Condition  2 is mass percent of C
 Condition  3 is mass percent of MN
 Condition  4 is mass percent of SI
 Condition  5 is mass percent of CR
 Condition  6 is mass percent of NI
 Condition  7 is mass percent of MO
 Condition  8 is mass percent of CU
 Condition  9 is mass percent of AL
 Condition 10 is mass percent of N
Give the number of the condition to vary /1/: 1
Minimum value (C) /800/: 650
Maximum value (C) /1800/: 1200

 The second axis can be another of the conditions above and you will then
 calculate a phase diagram.
 Or you may want to plot how some other quantities depend on the selected
 condition and you will then calculate a  "property" diagram.

 In addition to the conditions above you may use these selected
 dependent quantities on the vertical axis:
 Dependent 11 is mass fraction of all phases
 Dependent 12 is composition of a phase
 Dependent 13 is the fraction of a component in all phases
 (In the post processor you may select many other quantities)
Give the number of the quantity on second axis /11/: 11 tcex41
 No initial equilibrium, using default
 Step will start from axis value    1329.15
...OK

 Phase Region from    1329.15     for:
     ALN
     FCC_A1
 Global check of removing phase at  1.38422E+03
 Calculated     8 equilibria

 Phase Region from    1384.22     for:
     FCC_A1
 Global test at  1.45915E+03 .... OK
 Terminating at    1473.15
 Calculated    13 equilibria

 Phase Region from    1329.15     for:
     ALN
     FCC_A1
 Global test at  1.24915E+03 .... OK
 Global test at  1.14915E+03 .... OK
 Global check of adding phase at  1.07227E+03
 Calculated    28 equilibria

 Phase Region from    1072.27     for:
     ALN
     BCC_A2
     FCC_A1
 Global test at  9.99150E+02 .... OK
 Global check of adding phase at  9.98511E+02
 Calculated    11 equilibria

 Phase Region from    998.511     for:
     ALN
     BCC_A2
     FCC_A1
     M7C3
 Global check of adding phase at  9.96944E+02
 Calculated     3 equilibria

 Phase Region from    996.944     for:
     ALN
     BCC_A2
     CEMENTITE
     FCC_A1
     M7C3
 Global check of removing phase at  9.95944E+02
 Calculated     3 equilibria

 Phase Region from    995.944     for:
     ALN
     BCC_A2
     CEMENTITE
     FCC_A1
 Global check of removing phase at  9.68325E+02
 Calculated     6 equilibria
```

```
Phase Region from    968.325     for:
    ALN
    BCC_A2
    CEMENTITE
Global check of adding phase at  9.45779E+02
Calculated      5 equilibria

Phase Region from    945.779     for:
    ALN
    BCC_A2
    CEMENTITE
    M7C3
Terminating at    923.150
Calculated      6 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex41\tcex
41.POLY3

 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes

  ... the command in full is REINITIATE_PLOT_SETTINGS

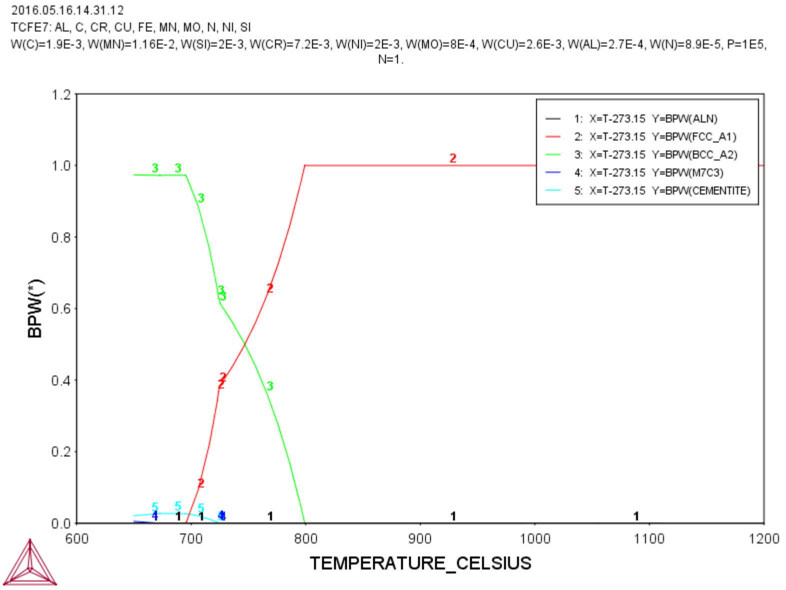
 POSTPROCESSOR VERSION 3.2


Setting automatic diagram axes

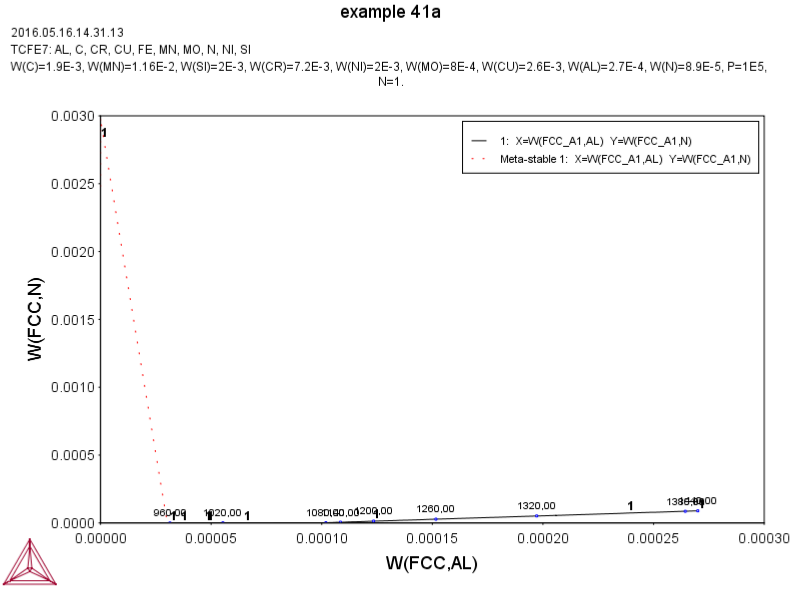
  ... the command in full is SET_AUTOMATIC_DIAGRAM_A

Setting automatic diagram axes

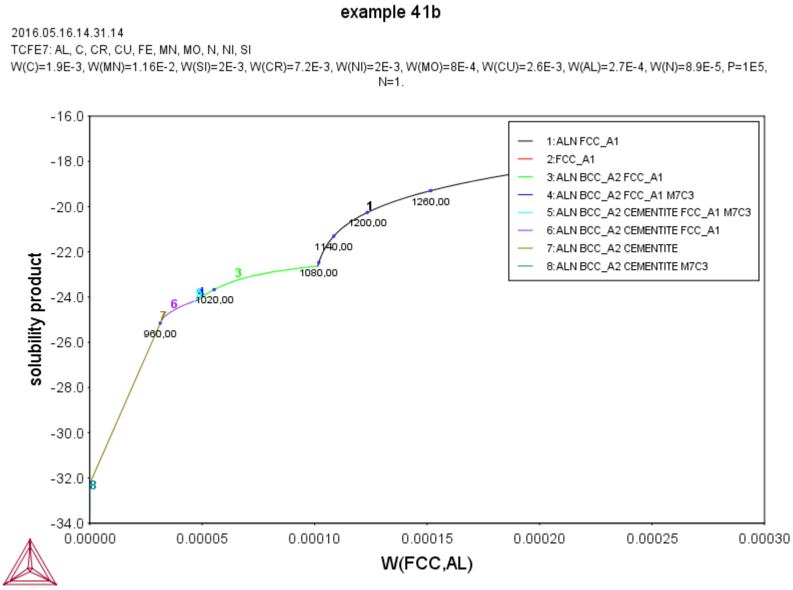
  ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a x w(fcc,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(fcc,n)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-d-a z t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 1250 1350
   ... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 41a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Now let's go back to POLY3 and enter a function
POST: @@ corresponding to the solubillity product
POST: back
POLY_3: enter fun
   ... the command in full is ENTER_SYMBOL
Name: sp
Function: log(w(fcc,al)*w(fcc,n));
POLY_3:
POLY_3: @@ Finally, let's go back to POST and plot the entered function
POLY_3: post
POST:
POST: s-d-a y sp
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-t-s y n solubility product
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: set-title example 41b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex42

```
About Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex42\tcex42.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Paraequilibrium calculation - Formation of Para-pearlite - Isopleth
SYS: @@
SYS: @@ Fe-Mn-C system at 2.5%Mn Mass u-fraction
SYS: @@
SYS: set-log ex42,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw tcfe7
   ... the command in full is SWITCH_DATABASE
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE7: d-sys fe c mn
   ... the command in full is DEFINE_SYSTEM
 FE                      C                       MN
   DEFINED
TDB_TCFE7: rej ph gra m5c2
   ... the command in full is REJECT
 GRAPHITE                M5C2  REJECTED
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

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  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
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  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
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  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C-FE-MO'
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       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'A. Markstrom, Thermo-Calc software AB, 2011'
 -OK-
TDB_TCFE7: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: @@
POLY_3: @@ To work with u-fractions, simply set the status of component C to SPECIAL
POLY_3: @@
POLY_3: c-s com c
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: special
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       SPECIAL   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 M7C3                    ENTERED      0.000000E+00    0.000000E+00
 M23C6                   ENTERED      0.000000E+00    0.000000E+00
 LAVES_PHASE_C14         ENTERED      0.000000E+00    0.000000E+00
 KSI_CARBIDE             ENTERED      0.000000E+00    0.000000E+00
```

```
 KAPPA                   ENTERED      0.000000E+00    0.000000E+00
 HCP_A3                  ENTERED      0.000000E+00    0.000000E+00
 G_PHASE                 ENTERED      0.000000E+00    0.000000E+00
 FECN_CHI                ENTERED      0.000000E+00    0.000000E+00
 FE4N_LP1                ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                  ENTERED      0.000000E+00    0.000000E+00
 DIAMOND_FCC_A4          ENTERED      0.000000E+00    0.000000E+00
 CEMENTITE               ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                  ENTERED      0.000000E+00    0.000000E+00
 LIQUID                  ENTERED      0.000000E+00    0.000000E+00
 GAS                     ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 C   ENTERED    C3  ENTERED    C5  ENTERED    FE  ENTERED    VA  ENTERED
 C2  ENTERED    C4  ENTERED    C60 ENTERED    MN  ENTERED
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: s-c t=900 p=1e5 n=1 w(c)=0.002 w(mn)=0.025
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         13031 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=900, P=1E5, N=1, W(C)=2E-3, W(MN)=2.5E-2
 DEGREES OF FREEDOM 0

 Temperature    900.00 K (   626.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.54204E+01
 Total Gibbs energy -3.64282E+04,  Enthalpy  2.02873E+04,  Volume  7.24808E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2099E-03  2.0000E-03 1.8066E-01 -1.2805E+04 SER
 FE                      9.6562E-01  9.7500E-01 8.1690E-03 -3.5974E+04 SER
 MN                      2.5169E-02  2.5000E-02 2.3600E-04 -6.2496E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.6371E-01, Mass 5.3798E+01, Volume fraction 9.6995E-01  Mass fractions:
 FE  9.81636E-01  MN  1.83337E-02  C   3.07634E-05

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 3.6288E-02, Mass 1.6223E+00, Volume fraction 3.0048E-02  Mass fractions:
 FE  6.88481E-01  MN  2.44355E-01  C   6.71647E-02
POLY_3: s-a-v 1 w(c) 0 0.02
   ... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/: 2.5E-04
POLY_3: s-a-v 2 t 800 1200 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex42a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
 Working hard

 Phase region boundary   1 at:   2.500E-04  8.868E+02
     BCC_A2
     CEMENTITE
```

```
 ** FCC_A1
Calculated.                      3  equilibria

Phase region boundary   2 at:   1.756E-05  8.799E+02
    BCC_A2
 ** CEMENTITE
 ** FCC_A1

Phase region boundary   3 at:   1.756E-05  8.799E+02
    BCC_A2
 ** FCC_A1
Calculated                     18  equilibria

Phase region boundary   4 at:   1.756E-05  8.799E+02
    BCC_A2
 ** CEMENTITE
Calculated..                     10  equilibria
Terminating at axis limit.

Phase region boundary   5 at:   1.756E-05  8.799E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     34  equilibria

Phase region boundary   6 at:   6.887E-03  9.767E+02
 ** BCC_A2
 ** CEMENTITE
    FCC_A1

Phase region boundary   7 at:   6.887E-03  9.767E+02
 ** CEMENTITE
    FCC_A1
Calculated..                     37  equilibria
Terminating at axis limit.

Phase region boundary   8 at:   6.887E-03  9.767E+02
 ** BCC_A2
    FCC_A1
Calculated                     47  equilibria

Phase region boundary   9 at:   6.887E-03  9.767E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1
Calculated..                     54  equilibria
Terminating at axis limit.

Phase region boundary  10 at:   1.756E-05  8.799E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     85  equilibria
Terminating at axis limit.

Phase region boundary  11 at:   2.500E-04  8.868E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     81  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  12 at:   6.750E-03  9.510E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     29  equilibria
Terminating at known equilibrium

Phase region boundary  13 at:   6.750E-03  9.510E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     55  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  14 at:   1.325E-02  9.678E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     57  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   1.325E-02  9.678E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     29  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   3.686E-06  8.100E+02
    BCC_A2
 ** CEMENTITE
Calculated..                      3  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  17 at:   3.686E-06  8.100E+02
    BCC_A2
 ** CEMENTITE
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   1.975E-02  9.759E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     80  equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   1.975E-02  9.759E+02
    BCC_A2
    CEMENTITE
```

```
 ** FCC_A1
Calculated..                       3  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   1.114E-03  9.367E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                       8  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   1.114E-03  9.367E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                      26  equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   4.017E-03  9.367E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                      17  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   4.017E-03  9.367E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                      66  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   1.018E-03  1.063E+03
 ** BCC_A2
    FCC_A1
Calculated.                      32  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   1.018E-03  1.063E+03
 ** BCC_A2
    FCC_A1
Calculated                      17  equilibria

Phase region boundary  26 at:   9.139E-03  1.063E+03
 ** CEMENTITE
    FCC_A1
Calculated.                      10  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   9.139E-03  1.063E+03
 ** CEMENTITE
    FCC_A1
Calculated..                      28  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:   1.283E-02  1.190E+03
 ** CEMENTITE
    FCC_A1
Calculated.                      34  equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   1.283E-02  1.190E+03
 ** CEMENTITE
    FCC_A1
Calculated..                       4  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  30 at:   2.500E-04  1.081E+03
 ** BCC_A2
    FCC_A1
Calculated                       4  equilibria

Phase region boundary  31 at:   2.500E-04  1.081E+03
 ** BCC_A2
    FCC_A1
Calculated.                      28  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   6.750E-03  9.783E+02
 ** BCC_A2
    FCC_A1
Calculated                      30  equilibria

Phase region boundary  33 at:   6.750E-03  9.783E+02
 ** BCC_A2
    FCC_A1
Calculated.                       2  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   1.325E-02  9.803E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1
Calculated.                      27  equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   1.325E-02  9.803E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1
Calculated..                      29  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  36 at:   1.283E-02  1.190E+03
 ** CEMENTITE
    FCC_A1
Calculated.                      34  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   1.283E-02  1.190E+03
 ** CEMENTITE
```

```
     FCC_A1
 Calculated..                      4  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

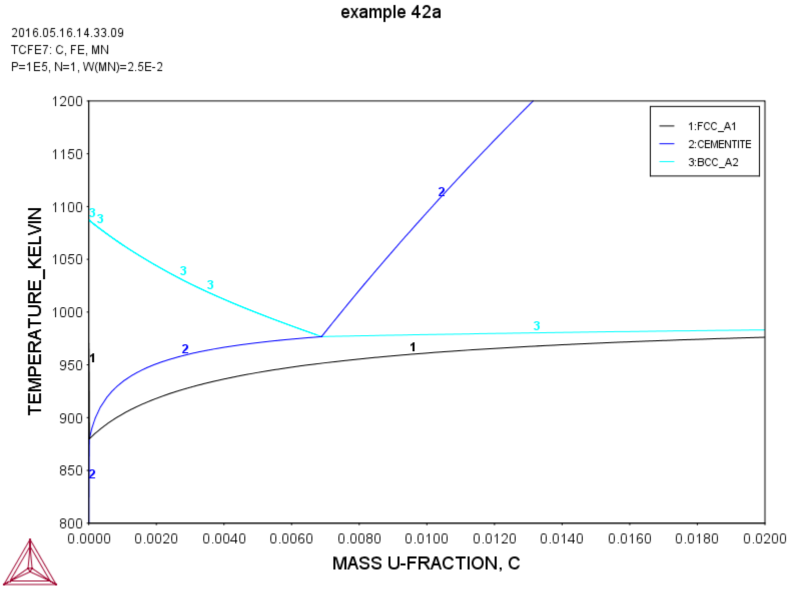
 Phase region boundary  38 at:   1.975E-02  9.830E+02
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated.                      53  equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   1.975E-02  9.830E+02
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated..                      3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex42\tcex
 42a.POLY3
 CPU time for mapping                      7  seconds
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-lab e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-text x n MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-title example 42a
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: make tcex42 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
POST: back
POLY_3: read tcex42a
   ... the command in full is READ_WORKSPACES
POLY_3: s-a-v 1 t 800 1200 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex42b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824    4.977501E-02    6.609390E-04   -2.303643E-01
   8.900000E+02    0.161    0.839    5.421135E-02    6.889794E-04   -1.689777E-02
   8.800000E+02    0.148    0.852    5.872152E-02    7.140931E-04    1.943989E-01
   8.700000E+02    0.137    0.863    6.329608E-02    7.362105E-04    4.040959E-01
   8.600000E+02    0.127    0.873    6.792661E-02    7.552871E-04    6.126989E-01
   8.500000E+02    0.119    0.881    7.260558E-02    7.713010E-04    8.206607E-01
   8.400000E+02    0.111    0.889    7.732629E-02    7.842505E-04    1.028392E+00
   8.300000E+02    0.105    0.895    8.208278E-02    7.941530E-04    1.236267E+00
   8.200000E+02    0.099    0.901    8.686971E-02    8.010431E-04    1.444633E+00
   8.100000E+02    0.093    0.907    9.168236E-02    8.049714E-04    1.653814E+00
```

```
   8.000000E+02    0.089    0.911   9.651648E-02   8.060032E-04   1.864114E+00

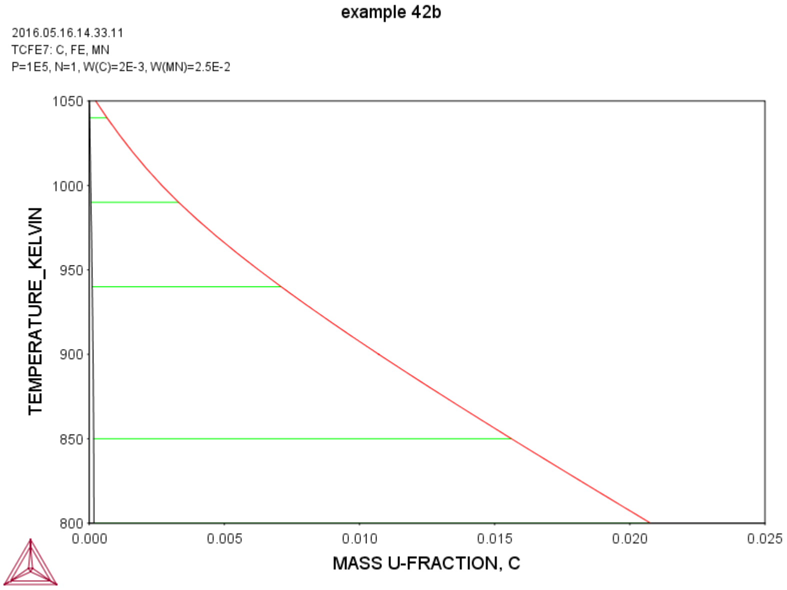
 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824   4.977501E-02   6.609390E-04  -2.303643E-01
   9.100000E+02    0.193    0.807   4.542308E-02   6.300692E-04  -4.466511E-01
   9.200000E+02    0.214    0.786   4.116735E-02   5.964982E-04  -6.665081E-01
   9.300000E+02    0.240    0.760   3.702095E-02   5.603899E-04  -8.908100E-01
   9.400000E+02    0.270    0.730   3.299845E-02   5.219482E-04  -1.120589E+00
   9.500000E+02    0.308    0.692   2.911596E-02   4.814238E-04  -1.357076E+00
   9.600000E+02    0.355    0.645   2.539121E-02   4.391211E-04  -1.601760E+00
   9.700000E+02    0.415    0.585   2.184354E-02   3.954079E-04  -1.856463E+00
   9.800000E+02    0.493    0.507   1.849394E-02   3.507265E-04  -2.123436E+00
   9.900000E+02    0.597    0.403   1.536496E-02   3.056079E-04  -2.405499E+00
   1.000000E+03    0.739    0.261   1.248054E-02   2.606888E-04  -2.706208E+00
   1.010000E+03    0.942    0.058   9.852896E-03   2.164281E-04  -3.031479E+00
   1.020000E+03    1.259   -0.259   7.420594E-03   1.715531E-04  -3.400603E+00
   1.030000E+03    1.821   -0.821   5.161354E-03   1.256551E-04  -3.846325E+00
   1.040000E+03    3.087   -2.087   3.063915E-03   7.858616E-05  -4.447717E+00
   1.050000E+03    8.516   -7.516   1.118169E-03   3.022614E-05  -5.532996E+00
 *** Buffer savend on file
 c:\jenkins\WORKSP~1\THERMO~1\examples\tcex42\TCEX42~2.POL

 *** ERROR     8 IN NS01AD
 *** Numerical error
POLY_3:
POLY_3: post

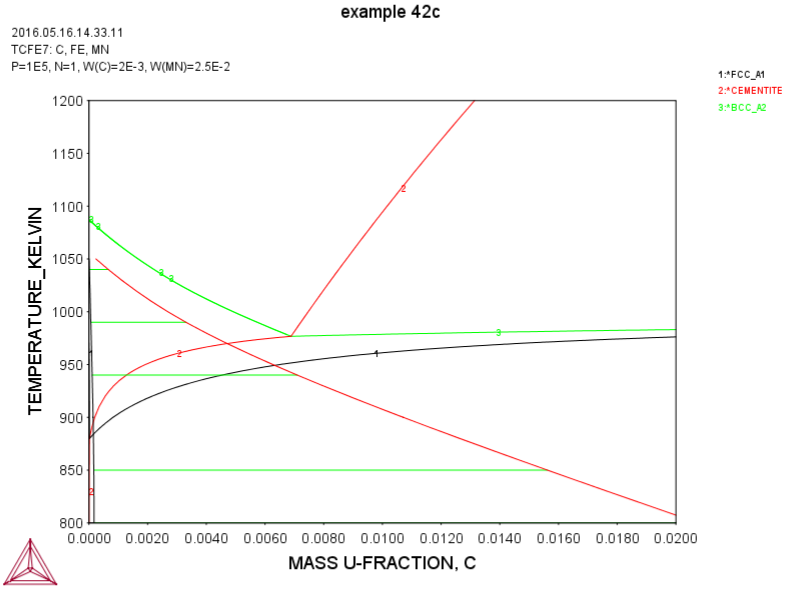
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 42b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: ap-e y tcex42
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.02
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 800 1200
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 42c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:Hit RETURN to continue
POST:
POST: back
POLY_3: read tcex42b
   ... the command in full is READ_WORKSPACES
POLY_3: s-c w(c)=0.01
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          13031 grid points in              0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time      0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=900, P=1E5, N=1, W(C)=1E-2, W(MN)=2.5E-2
 DEGREES OF FREEDOM 0

 Temperature    900.00 K (   626.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.38780E+01
 Total Gibbs energy -3.55135E+04,  Enthalpy  2.04087E+04,  Volume  7.05542E-06

 Component               Moles      W-Fraction  Activity   Potential  Ref.stat
 C                       4.4413E-02  1.0000E-02 2.8953E-01 -9.2753E+03 SER
 FE                      9.3131E-01  9.7500E-01 8.2548E-03 -3.5896E+04 SER
 MN                      2.4275E-02  2.5000E-02 1.0105E-04 -6.8844E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 8.2304E-01, Mass 4.5951E+01, Volume fraction 8.4974E-01  Mass fractions:
 FE  9.92487E-01  MN  7.46758E-03  C   4.52842E-05

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.7696E-01, Mass 7.9270E+00, Volume fraction 1.5026E-01  Mass fractions:
 FE  8.08018E-01  MN  1.24950E-01  C   6.70326E-02
POLY_3:
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    900.000     for:
     CEMENTITE
     FCC_A1
   9.000000E+02    0.932    0.068   2.554923E-02   3.333333E-01  -1.148376E+00
   8.900000E+02    0.929    0.071   2.453374E-02   3.333333E-01  -1.120519E+00
   8.800000E+02    0.926    0.074   2.353422E-02   3.333333E-01  -1.092268E+00
   8.700000E+02    0.923    0.077   2.255097E-02   3.333333E-01  -1.063621E+00
   8.600000E+02    0.920    0.080   2.158434E-02   3.333333E-01  -1.034574E+00
   8.500000E+02    0.917    0.083   2.063468E-02   3.333333E-01  -1.005126E+00
   8.400000E+02    0.915    0.085   1.970236E-02   3.333333E-01  -9.752721E-01
   8.300000E+02    0.912    0.088   1.878777E-02   3.333333E-01  -9.450113E-01
   8.200000E+02    0.909    0.091   1.789129E-02   3.333333E-01  -9.143405E-01
   8.100000E+02    0.907    0.093   1.701335E-02   3.333333E-01  -8.832577E-01
   8.000000E+02    0.904    0.096   1.615437E-02   3.333333E-01  -8.517606E-01

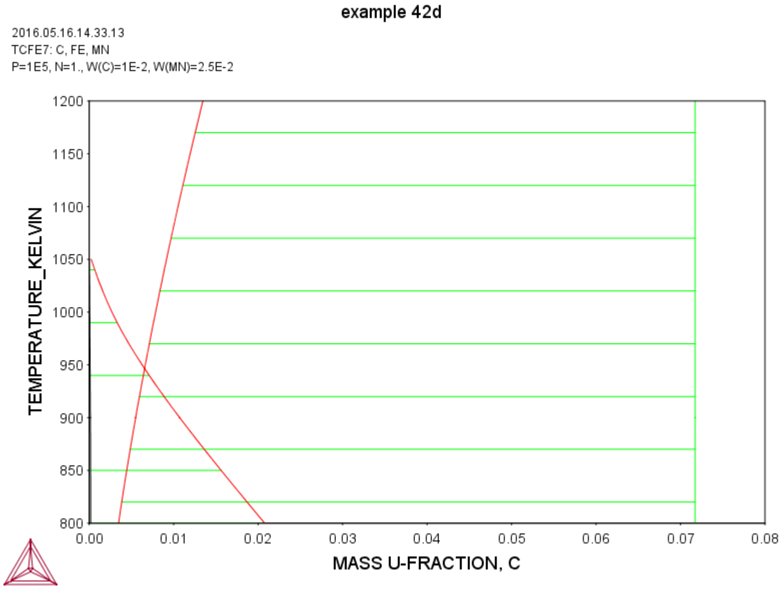
 Phase Region from    900.000     for:
     CEMENTITE
     FCC_A1
   9.000000E+02    0.932    0.068   2.554923E-02   3.333333E-01  -1.148376E+00
   9.100000E+02    0.935    0.065   2.658037E-02   3.333333E-01  -1.175842E+00
   9.200000E+02    0.938    0.062   2.762688E-02   3.333333E-01  -1.202921E+00
   9.300000E+02    0.942    0.058   2.868849E-02   3.333333E-01  -1.229615E+00
   9.400000E+02    0.945    0.055   2.976496E-02   3.333333E-01  -1.255928E+00
   9.500000E+02    0.948    0.052   3.085606E-02   3.333333E-01  -1.281861E+00
   9.600000E+02    0.952    0.048   3.196156E-02   3.333333E-01  -1.307420E+00
   9.700000E+02    0.955    0.045   3.308128E-02   3.333333E-01  -1.332605E+00
   9.800000E+02    0.959    0.041   3.421503E-02   3.333333E-01  -1.357420E+00
   9.900000E+02    0.963    0.037   3.536265E-02   3.333333E-01  -1.381869E+00
```

```
   1.000000E+03    0.966    0.034   3.652401E-02   3.333333E-01  -1.405953E+00
   1.010000E+03    0.970    0.030   3.769896E-02   3.333333E-01  -1.429677E+00
   1.020000E+03    0.974    0.026   3.888741E-02   3.333333E-01  -1.453041E+00
   1.030000E+03    0.978    0.022   4.008925E-02   3.333333E-01  -1.476050E+00
   1.040000E+03    0.982    0.018   4.130440E-02   3.333333E-01  -1.498705E+00
   1.050000E+03    0.986    0.014   4.253282E-02   3.333333E-01  -1.521010E+00
   1.060000E+03    0.991    0.009   4.377444E-02   3.333333E-01  -1.542967E+00
   1.070000E+03    0.995    0.005   4.502924E-02   3.333333E-01  -1.564577E+00
   1.080000E+03    0.999    0.001   4.629720E-02   3.333333E-01  -1.585844E+00
   1.090000E+03    1.004   -0.004   4.757831E-02   3.333333E-01  -1.606770E+00
   1.100000E+03    1.008   -0.008   4.887260E-02   3.333333E-01  -1.627357E+00
   1.110000E+03    1.013   -0.013   5.018009E-02   3.333333E-01  -1.647607E+00
   1.120000E+03    1.018   -0.018   5.150082E-02   3.333333E-01  -1.667522E+00
   1.130000E+03    1.023   -0.023   5.283486E-02   3.333333E-01  -1.687104E+00
   1.140000E+03    1.028   -0.028   5.418227E-02   3.333333E-01  -1.706354E+00
   1.150000E+03    1.033   -0.033   5.554314E-02   3.333333E-01  -1.725275E+00
   1.160000E+03    1.038   -0.038   5.691756E-02   3.333333E-01  -1.743868E+00
   1.170000E+03    1.043   -0.043   5.830566E-02   3.333333E-01  -1.762134E+00
   1.180000E+03    1.048   -0.048   5.970756E-02   3.333333E-01  -1.780075E+00
   1.190000E+03    1.054   -0.054   6.112340E-02   3.333333E-01  -1.797692E+00
   1.200000E+03    1.059   -0.059   6.255334E-02   3.333333E-01  -1.814987E+00
 *** Buffer savend on file
 c:\jenkins\WORKSP~1\THERMO~1\examples\tcex42\TCEX42~2.POL
POLY_3:
POLY_3: post

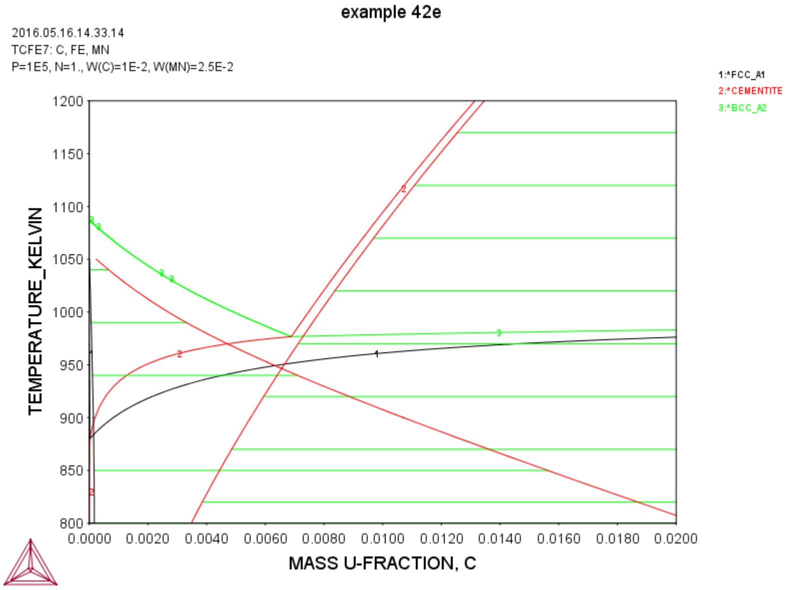
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-tit example 42d
   ... the command in full is SET_TITLE
POST: app-e n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: app-e y tcex42
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.02
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 42e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex43

About

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex43\tcex43.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Paraequilibrium calculation - Formation of Para-pearlite - Isothermal
SYS: @@
SYS: @@ Fe-Mn-C system at 700 C
SYS: @@
SYS: set-log ex43,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: d-mater
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Database /TCFE8/: tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 0.1
2nd alloying element: mn 2
Next alloying element:
Temperature (C) /1000/: 700
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M5C2                     KSI_CARBIDE
 A1_KAPPA                 KAPPA                    FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14          G_PHASE

Reject phase(s) /NONE/: graphite m5c2
 GRAPHITE                M5C2  REJECTED
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

 ........................................................

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 CEMENTITE                M23C6                    M7C3
 KSI_CARBIDE              A1_KAPPA                 KAPPA
 FE4N_LP1                 FECN_CHI                 LAVES_PHASE_C14
 G_PHASE

 ........................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'P. Franke, estimated parameter within SGTE, 2008; Fe-Mn-C'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C-FE-MO'
  'D. Connetable, J. Lacaze, P. Maugis and B. Sundman; Calphad, Vol. 32
      (2008), pp. 361-370; Al-C-Fe'
  'Thermo-Calc Software (2008): Volume data updated for TCFE6 database (TCFE
```

```
      v6, April, 2008).'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'Estimated parameter for solubility of C in Fe4N, 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'A. Markstrom, Thermo-Calc software AB, 2011'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         13031 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=973.15, W(C)=1E-3, W(MN)=2E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    973.15 K (   700.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.56256E+01
 Total Gibbs energy -4.11739E+04,  Enthalpy  2.46047E+04,  Volume  7.28123E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.6312E-03  1.0000E-03 1.2824E-01 -1.6618E+04 SER
 FE                      9.7512E-01  9.7900E-01 6.6199E-03 -4.0599E+04 SER
 MN                      2.0250E-02  2.0000E-02 1.0082E-04 -7.4457E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.8346E-01, Mass 4.3734E+01, Volume fraction 7.8722E-01  Mass fractions:
 FE  9.86998E-01  MN  1.29345E-02  C   6.74179E-05

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 2.1654E-01, Mass 1.1892E+01, Volume fraction 2.1278E-01  Mass fractions:
 FE  9.49585E-01  MN  4.59849E-02  C   4.42980E-03
POLY_3: @@
POLY_3: @@ change the status of component C to SPECIAL and work with u-fractions
POLY_3: @@
POLY_3: c-s comp c
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: spe
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         13031 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 w(c) 0 0.08
   ... the command in full is SET_AXIS_VARIABLE
Increment /.002/: 2.5E-04
POLY_3: s-a-v 2 w(mn) 0 0.1
   ... the command in full is SET_AXIS_VARIABLE
Increment /.0025/: .0025
POLY_3: l-a-v
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(C)                   Min: 0         Max: 8E-2      Inc: 2.5E-4
  Axis No 2: W(MN)                  Min: 0         Max: 0.1       Inc: 2.5E-3
POLY_3: sa tcex43a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
```

```
Generating start point  31
Generating start point  32

Phase region boundary   1 at:   3.082E-02  1.466E-02
    BCC_A2
 ** CEMENTITE
Calculated                     18  equilibria

Phase region boundary   2 at:   3.082E-02  1.466E-02
    BCC_A2
 ** CEMENTITE
Calculated.                     11  equilibria

Phase region boundary   3 at:   3.082E-02  3.943E-02
    BCC_A2
 ** CEMENTITE
 ** FCC_A1

Phase region boundary   4 at:   3.392E-03  1.781E-02
    BCC_A2
 ** FCC_A1
Calculated                     34  equilibria

Phase region boundary   5 at:   3.511E-02  5.220E-02
    CEMENTITE
 ** FCC_A1
Calculated..                     48  equilibria
Terminating at axis limit.

Phase region boundary   6 at:   3.082E-02  3.943E-02
    BCC_A2
 ** CEMENTITE
Calculated                     27  equilibria

Phase region boundary   7 at:   3.082E-02  1.466E-02
    BCC_A2
 ** CEMENTITE
Calculated                     18  equilibria

Phase region boundary   8 at:   3.082E-02  1.466E-02
    BCC_A2
 ** CEMENTITE
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary   9 at:   3.082E-02  2.813E-03
    BCC_A2
 ** CEMENTITE
Calculated                     10  equilibria

Phase region boundary  10 at:   3.082E-02  2.813E-03
    BCC_A2
 ** CEMENTITE
Calculated.                     16  equilibria
Terminating at known equilibrium

Phase region boundary  11 at:   3.082E-02  1.549E-03
    BCC_A2
 ** CEMENTITE
Calculated                     13  equilibria

Phase region boundary  12 at:   3.082E-02  1.549E-03
    BCC_A2
 ** CEMENTITE
Calculated.                     17  equilibria
Terminating at known equilibrium

Phase region boundary  13 at:   3.585E-01  2.500E-03
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated                     22  equilibria

Phase region boundary  14 at:   3.585E-01  2.500E-03
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated.                    133  equilibria

Phase region boundary  15 at:   3.604E-01  3.323E-01
    CEMENTITE
 ** DIAMOND_FCC_A4
 ** M7C3

Phase region boundary  16 at:   8.213E-02  4.124E-01
    CEMENTITE
 ** M7C3

Phase region boundary  17 at:   4.027E-01  4.984E-01
    DIAMOND_FCC_A4
 ** M7C3

Phase region boundary  18 at:   3.604E-01  3.323E-01
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated                    142  equilibria

Phase region boundary  19 at:   3.585E-01  2.500E-03
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated                     22  equilibria

Phase region boundary  20 at:   3.585E-01  2.500E-03
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated.                    133  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   4.549E-04  4.437E-02
    BCC_A2
 ** FCC_A1
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   4.549E-04  4.437E-02
    BCC_A2
 ** FCC_A1
Calculated                     13  equilibria
```

```
Phase region boundary  23 at:   3.587E-01  3.417E-02
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated                     26  equilibria

Phase region boundary  24 at:   3.587E-01  3.417E-02
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated.                    121  equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   1.375E-04  4.677E-02
 ** BCC_A2
    FCC_A1
Calculated.                     19  equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   1.375E-04  4.677E-02
 ** BCC_A2
    FCC_A1
Calculated                     19  equilibria

Phase region boundary  27 at:   3.588E-01  6.583E-02
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated                     38  equilibria

Phase region boundary  28 at:   3.588E-01  6.583E-02
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated.                    108  equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   3.488E-02  1.652E-01
 ** CEMENTITE
    FCC_A1
Calculated.                     47  equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   3.488E-02  1.652E-01
 ** CEMENTITE
    FCC_A1
Calculated..                      3  equilibria
Terminating at axis limit.

Phase region boundary  31 at:   3.488E-02  1.677E-01
 ** CEMENTITE
    FCC_A1
Calculated.                     48  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   1.264E-04  4.685E-02
 ** BCC_A2
    FCC_A1
Calculated                      9  equilibria

Phase region boundary  33 at:   1.264E-04  4.685E-02
 ** BCC_A2
    FCC_A1
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   3.498E-02  1.113E-01
 ** CEMENTITE
    FCC_A1
Calculated.                     25  equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   3.498E-02  1.113E-01
 ** CEMENTITE
    FCC_A1
Calculated..                     25  equilibria
Terminating at axis limit.

Phase region boundary  36 at:   3.488E-02  1.688E-01
 ** CEMENTITE
    FCC_A1
Calculated.                     48  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   3.506E-02  7.604E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     11  equilibria
Terminating at known equilibrium

Phase region boundary  38 at:   3.506E-02  7.604E-02
 ** CEMENTITE
    FCC_A1
Calculated..                     39  equilibria
Terminating at axis limit.

Phase region boundary  39 at:   3.488E-02  1.685E-01
 ** CEMENTITE
    FCC_A1
Calculated.                     48  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   3.590E-01  9.750E-02
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated                     42  equilibria

Phase region boundary  41 at:   3.590E-01  9.750E-02
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated.                     95  equilibria
Terminating at known equilibrium

Phase region boundary  42 at:   3.590E-01  9.750E-02
    CEMENTITE
 ** DIAMOND_FCC_A4
Calculated                     42  equilibria

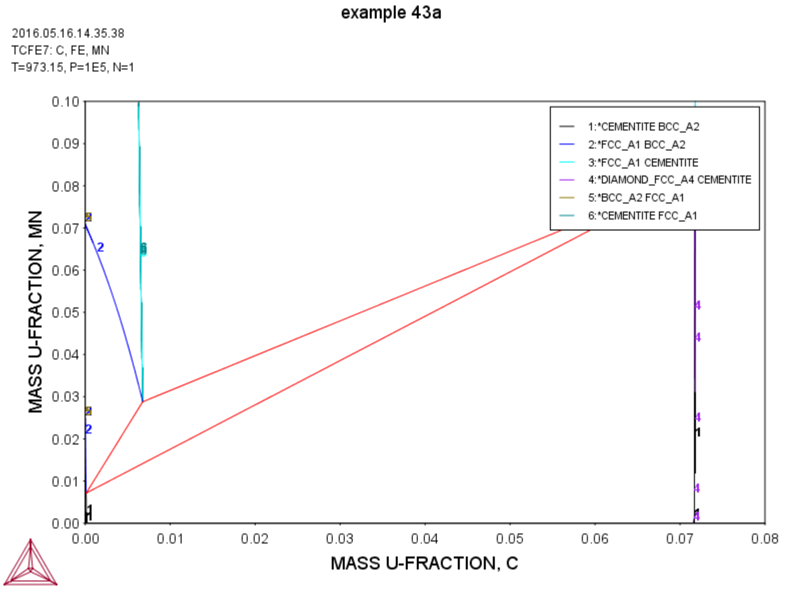
Phase region boundary  43 at:   3.590E-01  9.750E-02
```

```
     CEMENTITE
   ** DIAMOND_FCC_A4
 Calculated.                      95  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex43\tcex
 43a.POLY3
 CPU time for mapping                        4  seconds
POLY_3:
POLY_3: post

   POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-lab e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 43a
POST: s-ax-text x N MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N MASS U-FRACTION, MN
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: make tcex43 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: b
   ... the command in full is BACK
POLY_3: read tcex43a
   ... the command in full is READ_WORKSPACES
POLY_3: s-a-v 1 w(mn) 0 0.1
   ... the command in full is SET_AXIS_VARIABLE
Increment /.0025/: .0025
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex43b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from   0.200000E-01 for:
     BCC_A2
     FCC_A1
   2.000000E-02    0.165    0.835   2.571485E-02   4.910396E-04  -1.652126E+00
   1.750000E-02    0.148    0.852   2.818000E-02   5.485823E-04  -1.524121E+00
   1.500000E-02    0.135    0.865   3.063880E-02   6.079802E-04  -1.404111E+00
   1.250000E-02    0.123    0.877   3.309067E-02   6.692476E-04  -1.290883E+00
   1.000000E-02    0.113    0.887   3.553566E-02   7.324129E-04  -1.183465E+00
   7.500000E-03    0.104    0.896   3.797362E-02   7.974991E-04  -1.081091E+00
   5.000000E-03    0.096    0.904   4.040445E-02   8.645295E-04  -9.831360E-01
   2.500000E-03    0.089    0.911   4.282805E-02   9.335273E-04  -8.890905E-01
   2.500000E-09    0.082    0.918   4.524437E-02   1.004515E-03  -7.985285E-01

 Phase Region from   0.200000E-01 for:
     BCC_A2
     FCC_A1
   2.000000E-02    0.165    0.835   2.571485E-02   4.910396E-04  -1.652126E+00
   2.250000E-02    0.185    0.815   2.324342E-02   4.353248E-04  -1.789740E+00
   2.500000E-02    0.209    0.791   2.076601E-02   3.814145E-04  -1.939115E+00
   2.750000E-02    0.241    0.759   1.828295E-02   3.292857E-04  -2.103233E+00
   3.000000E-02    0.282    0.718   1.579466E-02   2.789151E-04  -2.286396E+00
   3.250000E-02    0.338    0.662   1.330158E-02   2.302795E-04  -2.495141E+00
   3.500000E-02    0.420    0.580   1.080428E-02   1.833559E-04  -2.740125E+00
   3.750000E-02    0.552    0.448   8.303377E-03   1.381213E-04  -3.040528E+00
   4.000000E-02    0.798    0.202   5.799614E-03   9.455272E-05  -3.436595E+00
   4.250000E-02    1.418   -0.418   3.293836E-03   5.262739E-05  -4.039594E+00
```

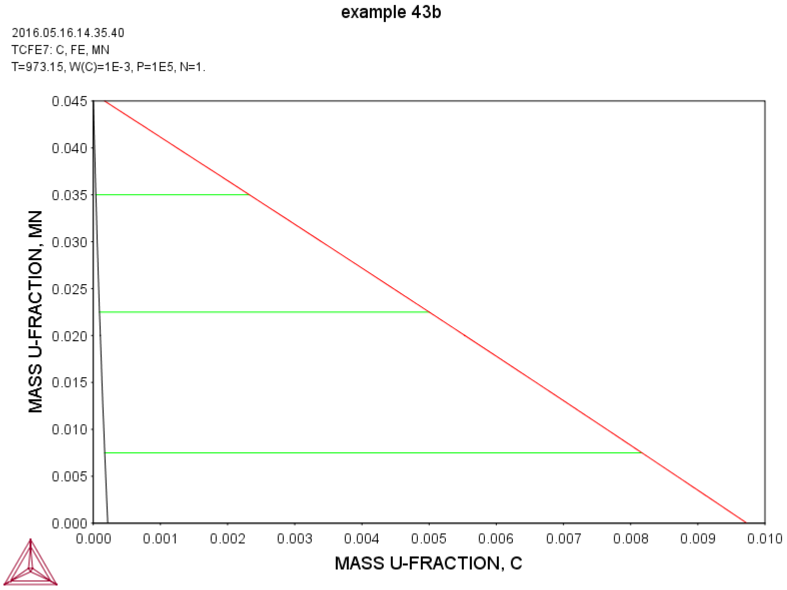
```
   4.500000E-02    5.984   -4.984   7.870255E-04   1.232263E-05  -5.508458E+00
 *** Buffer savend on file
 c:\jenkins\WORKSP~1\THERMO~1\examples\tcex43\TCEX43~2.POL

 *** ERROR     3 IN NS01AD
 *** Numerical error
POLY_3: po
   ... the command in full is POST

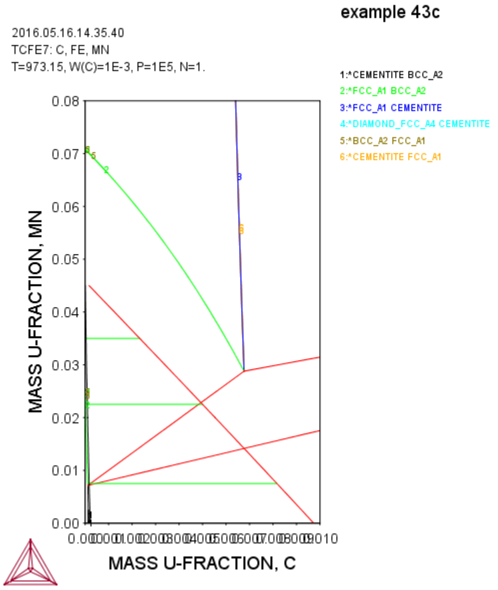
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y w(*,mn)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 43b
POST: s-ax-text x N MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N MASS U-FRACTION, MN
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: app y tcex43
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.01
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.08
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 43c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
```

```
POST: b
   ... the command in full is BACK
POLY_3: read tcex43b
   ... the command in full is READ_WORKSPACES
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=973.15, W(C)=1E-3, W(MN)=2E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY_3: s-c w(c)=0.008 w(mn)=0.07
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         13031 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=973.15, W(C)=8E-3, W(MN)=7E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    973.15 K (   700.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.42144E+01
 Total Gibbs energy -4.19857E+04,  Enthalpy  2.75863E+04,  Volume  7.10872E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        3.5823E-02  8.0000E-03 1.8345E-01 -1.3721E+04 SER
 FE                       8.9565E-01  9.3000E-01 6.4227E-03 -4.0844E+04 SER
 MN                       6.8530E-02  7.0000E-02 1.4208E-04 -7.1681E+04 SER

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.7022E-01, Mass 5.2881E+01, Volume fraction 9.7477E-01  Mass fractions:
 FE  9.26648E-01  MN  6.69068E-02  C   6.44559E-03

 CEMENTITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 2.9780E-02, Mass 1.3330E+00, Volume fraction 2.5229E-02  Mass fractions:
 FE  7.62802E-01  MN  1.70116E-01  C   6.70826E-02
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 NP(FCC_A1) =   0.9928 with U-fractions C  =  3.50068E-02
 NP(CEMENTITE) =   0.0072 with U-fractions C  =  3.33333E-01
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

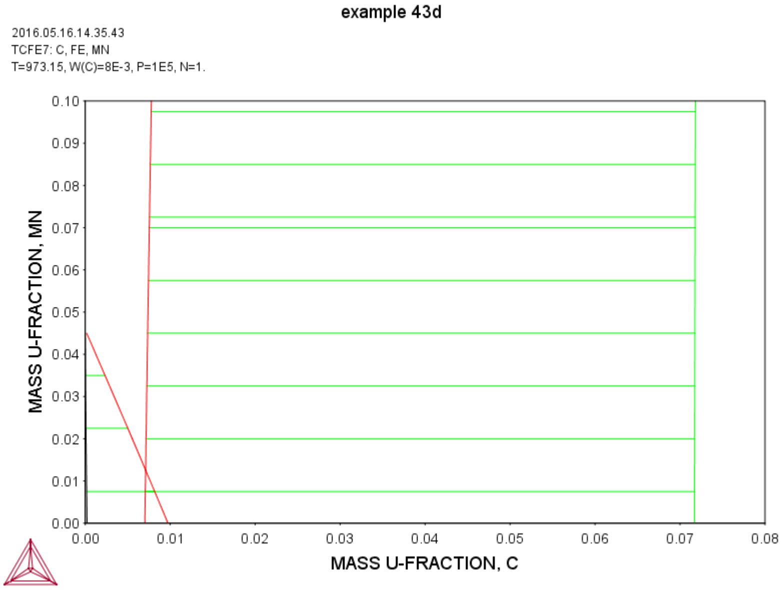
 Phase Region from   0.700000E-01 for:
     CEMENTITE
     FCC_A1
   7.000000E-02    0.993    0.007   3.500676E-02   3.333333E-01  -1.512238E+00
   6.750000E-02    0.993    0.007   3.491610E-02   3.333333E-01  -1.502576E+00
   6.500000E-02    0.992    0.008   3.482586E-02   3.333333E-01  -1.492928E+00
   6.250000E-02    0.992    0.008   3.473603E-02   3.333333E-01  -1.483293E+00
   6.000000E-02    0.992    0.008   3.464662E-02   3.333333E-01  -1.473672E+00
   5.750000E-02    0.991    0.009   3.455761E-02   3.333333E-01  -1.464066E+00
   5.500000E-02    0.991    0.009   3.446901E-02   3.333333E-01  -1.454473E+00
   5.250000E-02    0.991    0.009   3.438081E-02   3.333333E-01  -1.444894E+00
   5.000000E-02    0.990    0.010   3.429302E-02   3.333333E-01  -1.435329E+00
   4.750000E-02    0.990    0.010   3.420563E-02   3.333333E-01  -1.425778E+00
   4.500000E-02    0.990    0.010   3.411864E-02   3.333333E-01  -1.416242E+00
   4.250000E-02    0.990    0.010   3.403205E-02   3.333333E-01  -1.406719E+00
   4.000000E-02    0.989    0.011   3.394585E-02   3.333333E-01  -1.397211E+00
   3.750000E-02    0.989    0.011   3.386005E-02   3.333333E-01  -1.387717E+00
   3.500000E-02    0.989    0.011   3.377464E-02   3.333333E-01  -1.378237E+00
   3.250000E-02    0.988    0.012   3.368963E-02   3.333333E-01  -1.368772E+00
   3.000000E-02    0.988    0.012   3.360500E-02   3.333333E-01  -1.359321E+00
   2.750000E-02    0.988    0.012   3.352076E-02   3.333333E-01  -1.349884E+00
   2.500000E-02    0.988    0.012   3.343690E-02   3.333333E-01  -1.340462E+00
   2.250000E-02    0.987    0.013   3.335343E-02   3.333333E-01  -1.331054E+00
   2.000000E-02    0.987    0.013   3.327034E-02   3.333333E-01  -1.321660E+00
   1.750000E-02    0.987    0.013   3.318763E-02   3.333333E-01  -1.312282E+00
   1.500000E-02    0.987    0.013   3.310530E-02   3.333333E-01  -1.302918E+00
   1.250000E-02    0.986    0.014   3.302335E-02   3.333333E-01  -1.293568E+00
   1.000000E-02    0.986    0.014   3.294177E-02   3.333333E-01  -1.284233E+00
   7.500000E-03    0.986    0.014   3.286057E-02   3.333333E-01  -1.274913E+00
   5.000000E-03    0.985    0.015   3.277974E-02   3.333333E-01  -1.265607E+00
   2.500000E-03    0.985    0.015   3.269928E-02   3.333333E-01  -1.256316E+00
   2.500000E-09    0.985    0.015   3.261919E-02   3.333333E-01  -1.247040E+00

 Phase Region from   0.700000E-01 for:
     CEMENTITE
     FCC_A1
   7.000000E-02    0.993    0.007   3.500676E-02   3.333333E-01  -1.512238E+00
   7.250000E-02    0.993    0.007   3.509783E-02   3.333333E-01  -1.521914E+00
   7.500000E-02    0.993    0.007   3.518931E-02   3.333333E-01  -1.531604E+00
   7.750000E-02    0.994    0.006   3.528122E-02   3.333333E-01  -1.541307E+00
   8.000000E-02    0.994    0.006   3.537355E-02   3.333333E-01  -1.551024E+00
   8.250000E-02    0.994    0.006   3.546630E-02   3.333333E-01  -1.560755E+00
   8.500000E-02    0.995    0.005   3.555948E-02   3.333333E-01  -1.570499E+00
   8.750000E-02    0.995    0.005   3.565309E-02   3.333333E-01  -1.580257E+00
   9.000000E-02    0.995    0.005   3.574712E-02   3.333333E-01  -1.590028E+00
```

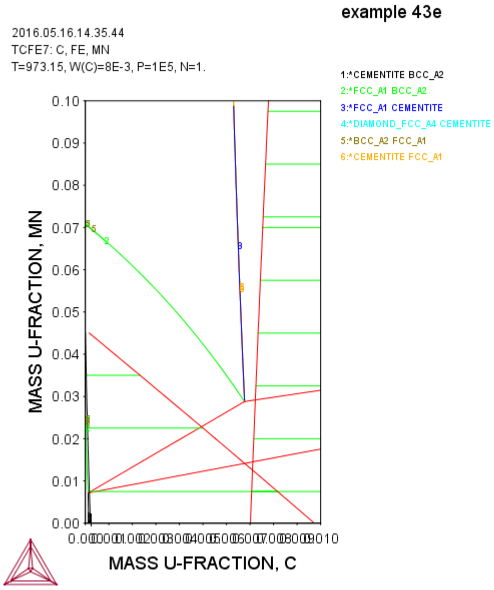
```
   9.250000E-02    0.996    0.004   3.584159E-02   3.333333E-01  -1.599812E+00
   9.500000E-02    0.996    0.004   3.593649E-02   3.333333E-01  -1.609610E+00
   9.750000E-02    0.996    0.004   3.603182E-02   3.333333E-01  -1.619421E+00
   1.000000E-01    0.997    0.003   3.612760E-02   3.333333E-01  -1.629246E+00
 *** Buffer savend on file
 c:\jenkins\WORKSP~1\THERMO~1\examples\tcex43\TCEX43~2.POL
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y w(*,mn)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 43d
POST: s-ax-text x N MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N MASS U-FRACTION, MN
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: app-e n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST:
POST: s-s x n 0 0.01
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.10
   ... the command in full is SET_SCALING_STATUS
POST: app-e y tcex43
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 43e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
```

POST:

tcex44

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex44\tcex44.TCM" set-echo
SYS: @@
SYS: @@ Exploring the usage of variables and functions. Proof strength for an austenitic stainless steel at elevated temperatures.
SYS: @@
SYS: @@
SYS: @@ Exploring the usage of variables and functions in order to predict
SYS: @@ properties e.g. Proof strength for an austenitic stainless
SYS: @@ steel (20-550C)
SYS:
SYS: go da
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw tcfe7
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE7: def-sys
ELEMENTS: fe c si mn cr ni mo cu n
 FE                      C                       SI
 MN                      CR                      NI
 MO                      CU                      N
   DEFINED
TDB_TCFE7: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

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      Mo-C-N, Fe-Mo-C-N'
  'D. Connetable, J. Lacaze, P. Maugis and B. Sundman; Calphad, Vol. 32
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  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
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      (1986); CR-FE-MO'
  'Unassessed parameter, linear combination of unary data; (MU, SIGMA)'
  'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
  'N. Saunders, COST 507 Report (1998); Al-Cu'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
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  'I. Ansara, unpublished work (1991); Cr-Si'
  'A. Bolcavage and U.R. Kattner, J. Phase Equil., 2, (1996); Nb-Ni'
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  'A. Markstrom, Thermo-Calc software AB, 2011'
 -OK-
TDB_TCFE7:
TDB_TCFE7: go p-3

 POLY version  3.32
POLY_3:
POLY_3: s-c p=1e5,n=1,t=1353
POLY_3: s-c w(c)=0.0009,w(n)=0.0007,w(cr)=.246,w(ni)=0.2,w(mn)=0.013
POLY_3: s-c w(si)=0.013,w(cu)=0.0024,w(mo)=0.003
POLY_3: l-c
 P=1E5, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
    W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
 DEGREES OF FREEDOM 0
POLY_3: c-e
 Using global minimization procedure
Calculated         34286 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 P=1E5, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
    W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
 DEGREES OF FREEDOM 0

 Temperature   1353.00 K (  1079.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.44622E+01
 Total Gibbs energy -8.11772E+04,  Enthalpy  3.59088E+04,  Volume  7.33318E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.0809E-03  9.0000E-04 1.3125E-03 -7.4650E+04 SER
 CR                      2.5767E-01  2.4600E-01 2.7776E-03 -6.6217E+04 SER
 CU                      2.0569E-03  2.4000E-03 8.2084E-05 -1.0583E+05 SER
 FE                      5.0808E-01  5.2100E-01 1.1351E-03 -7.6283E+04 SER
```

```
 MN                        1.2887E-02  1.3000E-02 6.4085E-06 -1.3452E+05 SER
 MO                        1.7030E-03  3.0000E-03 6.2271E-05 -1.0894E+05 SER
 N                         2.7217E-03  7.0000E-04 1.5560E-07 -1.7635E+05 SER
 NI                        1.8559E-01  2.0000E-01 2.2145E-04 -9.4668E+04 SER
 SI                        2.5209E-02  1.3000E-02 3.5318E-08 -1.9303E+05 SER

 FCC_A1                        Status ENTERED     Driving force  0.0000E+00
 Moles 9.9426E-01, Mass 5.4205E+01, Volume fraction 9.9495E-01  Mass fractions:
 FE  5.22729E-01  SI  1.30618E-02  CU  2.41140E-03
 CR  2.43674E-01  MN  1.30378E-02  N   7.03326E-03
 NI  2.00856E-01  MO  2.88542E-03  C   6.41161E-04

 M23C6                         Status ENTERED     Driving force  0.0000E+00
 Moles 5.7392E-03, Mass 2.5758E-01, Volume fraction 5.0456E-03  Mass fractions:
 CR  7.35501E-01  MO  2.71117E-02  N   0.00000E+00
 FE  1.57176E-01  NI  1.97963E-02  CU  0.00000E+00
 C   5.53701E-02  MN  5.04497E-03  SI  0.00000E+00
POLY_3:
POLY_3: @@ Define some variables
POLY_3: enter-symb
Constant, variable, function or table? /FUNCTION/: variable
Name: cc
Function: 100*w(fcc_a1,c)
&
POLY_3: ent var csi=100*w(fcc_a1,si);
POLY_3: ent var cmn=100*w(fcc_a1,mn);
POLY_3: ent var ccr=100*w(fcc_a1,cr);
POLY_3: ent var cni=100*w(fcc_a1,ni);
POLY_3: ent var cmo=100*w(fcc_a1,mo);
POLY_3: ent var ccu=100*w(fcc_a1,cu);
POLY_3: ent var cn=100*w(fcc_a1,n);
POLY_3: ent var cfe=100*w(fcc_a1,fe);
POLY_3: ent var cm23=100*bpw(m23c6);
POLY_3:
POLY_3: li-sy
 DEFINED FUNCTIONS AND VARIABLES%
    CC%=100*W(FCC_A1,C)
    CSI%=100*W(FCC_A1,SI)
    CMN%=100*W(FCC_A1,MN)
    CCR%=100*W(FCC_A1,CR)
    CNI%=100*W(FCC_A1,NI)
    CMO%=100*W(FCC_A1,MO)
    CCU%=100*W(FCC_A1,CU)
    CN%=100*W(FCC_A1,N)
    CFE%=100*W(FCC_A1,FE)
    CM23%=100*BPW(M23C6)
POLY_3:
POLY_3: eval
Name(s): *
 CC=6.4116133E-2
 CSI=1.3061775
 CMN=1.3037802
 CCR=24.367392
 CNI=20.085632
 CMO=0.28854226
 CCU=0.24114047
 CN=7.0332636E-2
 CFE=52.272887
 CM23=0.47294685
POLY_3:
POLY_3: enter-symb
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: tc=t-273.15;
POLY_3:
POLY_3: @@ Enter empirical parameters as function of temperature
POLY_3: ent func bc=575-0.3686*tc;
POLY_3: ent func bsi=24.76+1.129e-4*tc*tc-0.09*tc;
POLY_3: ent func bmn=-1.4-0.007*tc;
POLY_3: ent func bcr=0.3-tc*7e-4;
POLY_3: ent func bni=5.3-tc*3.3e-3;
POLY_3: ent func bmo=6-tc*3.3e-3;
POLY_3: ent func bcu=-14+0.0116*tc;
POLY_3: ent func bn=937-2.74e-6*tc*tc*tc+5.24e-3*tc*tc-3.08*tc;
POLY_3: ent func bm23=48+0.0135*tc;
POLY_3: ent func at=1.68+4.248e-6*tc*tc-4.33e-3*tc;
POLY_3:
POLY_3: li-symb *
 DEFINED FUNCTIONS AND VARIABLES%
    CC%=100*W(FCC_A1,C)
    CSI%=100*W(FCC_A1,SI)
    CMN%=100*W(FCC_A1,MN)
    CCR%=100*W(FCC_A1,CR)
    CNI%=100*W(FCC_A1,NI)
    CMO%=100*W(FCC_A1,MO)
    CCU%=100*W(FCC_A1,CU)
    CN%=100*W(FCC_A1,N)
    CFE%=100*W(FCC_A1,FE)
    CM23%=100*BPW(M23C6)
    TC=T-273.15
    BC=575-.3686*TC
    BSI=24.76+1.129E-04*TC*TC-.09*TC
    BMN=-1.4-.007*TC
    BCR=.3-TC*7E-04
    BNI=5.3-TC*.0033
    BMO=6-TC*.0033
    BCU=-14+.0116*TC
    BN=937-2.74E-06*TC*TC*TC+.00524*TC*TC-3.08*TC
    BM23=48+.0135*TC
    AT=1.68+4.248E-06*TC*TC-.00433*TC
POLY_3:
POLY_3: eval
Name(s): *
 CC=6.4116133E-2
 CSI=1.3061775
 CMN=1.3037802
 CCR=24.367392
 CNI=20.085632
 CMO=0.28854226
 CCU=0.24114047
 CN=7.0332636E-2
 CFE=52.272887
 CM23=0.47294685
 TC=1079.85
 BC=176.96729
```

```
 BSI=59.223483
 BMN=-8.95895
 BCR=-0.455895
 BNI=1.736495
 BMO=2.436495
 BCU=-1.47374
 BN=271.12745
 BM23=62.577975
 AT=1.9577404
POLY_3:
POLY_3: @@ Enter an empirical expression for the proof strength combining
POLY_3: @@ the variables and function parameters previuously entered.
POLY_3: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp1
Function: at+bc*cc+bsi*csi+bmn*cmn+bni*cni;
POLY_3:
POLY_3: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp2
Function: bcr*ccr+bmo*cmo+bcu*ccu+bn*cn+bm23*cm23;
POLY_3:
POLY_3: ent func rp02=rp1+rp2;
POLY_3:
POLY_3: eval
Name(s): *
 CC=6.4116133E-2
 CSI=1.3061775
 CMN=1.3037802
 CCR=24.367392
 CNI=20.085632
 CMO=0.28854226
 CCU=0.24114047
 CN=7.0332636E-2
 CFE=52.272887
 CM23=0.47294685
 TC=1079.85
 BC=176.96729
 BSI=59.223483
 BMN=-8.95895
 BCR=-0.455895
 BNI=1.736495
 BMO=2.436495
 BCU=-1.47374
 BN=271.12745
 BM23=62.577975
 AT=1.9577404
 RP1=113.85868
 RP2=37.903846
 RP02=151.76252
POLY_3:
POLY_3: @@ turn off the global minimization calculation and suspend
POLY_3: @@ all phases except fcc_a1#1. This will speed up the calculation
POLY_3: @@ and doesn't affect the results.
POLY_3: advanced
Which option? /STEP_AND_MAP/: glo
 Settings for global minimization:
   Use global minimization as much as possible /Y/: n,,,,
POLY_3:
POLY_3: c-s phase
Phase name(s): *
Status: /ENTERED/: sus
POLY_3:
POLY_3: c-s phase fcc_a1#1=enter 1
POLY_3:
POLY_3: s-c t=500
POLY_3: c-e
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
     7 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 P=1E5, N=1, T=500, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
    W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.44622E+01
 Total Gibbs energy -1.87430E+04,  Enthalpy  9.33796E+03,  Volume  7.00887E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.0809E-03  9.0000E-04 6.3735E-02 -1.1445E+04 SER
 CR                      2.5767E-01  2.4600E-01 2.3975E-01 -5.9371E+03 SER
 CU                      2.0569E-03  2.4000E-03 6.2527E-01 -1.9521E+03 SER
 FE                      5.0808E-01  5.2100E-01 3.3960E-02 -1.4062E+04 SER
 MN                      1.2887E-02  1.3000E-02 6.1504E-06 -4.9883E+04 SER
 MO                      1.7030E-03  3.0000E-03 6.4768E-02 -1.1378E+04 SER
 N                       2.7217E-03  7.0000E-04 5.4203E-14 -1.2699E+05 SER
 NI                      1.8559E-01  2.0000E-01 9.0077E-04 -2.9152E+04 SER
 SI                      2.5209E-02  1.3000E-02 1.2109E-15 -1.4279E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4462E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  5.21000E-01  SI  1.30000E-02  CU  2.40000E-03
 CR  2.46000E-01  MN  1.30000E-02  C   9.00000E-04
 NI  2.00000E-01  MO  3.00000E-03  N   7.00000E-04
POLY_3: l-st
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       ENTERED   SER
 CR                      ENTERED   SER
 CU                      ENTERED   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 MO                      ENTERED   SER
 N                       ENTERED   SER
 NI                      ENTERED   SER
 SI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
```

```
 FCC_A1                  ENTERED      0.000000E+00    1.000000E+00
 SUSPENDED PHASES:
 Z_PHASE SIGMA SIC SI3N4 R_PHASE P_PHASE PI NI3TI NBNI3 MU_PHASE MSI MN6N5
 MN6N4 MC_SHP MC_ETA M7C3 M6C M5SI3 M5C2 M3SI M3C2 M23C6 LAVES_PHASE_C14
 KSI_CARBIDE KAPPA HCP_A3#2 HCP_A3 G_PHASE GRAPHITE FECN_CHI FE8SI2C FE4N_LP1
 FE2SI FCC_A1#2 DIAMOND_FCC_A4 CR3SI CHI_A12 CEMENTITE BCC_A2 AL4C3 LIQUID GAS
 *** STATUS FOR ALL SPECIES
 C        ENTERED    C3       ENTERED    C6N1     ENTERED    N        ENTERED
 C1N1     ENTERED    C3N1     ENTERED    C6N2     ENTERED    N2       ENTERED
 C1N2_CNN ENTERED    C4       ENTERED    C9N1     ENTERED    N3       ENTERED
 C1N2_NCN ENTERED    C4N1     ENTERED    CR       ENTERED    NI       ENTERED
 C2       ENTERED    C4N2     ENTERED    CU       ENTERED    SI       ENTERED
 C2N1_CCN ENTERED    C5       ENTERED    FE       ENTERED    SI3N4    ENTERED
 C2N1_CNC ENTERED    C5N1     ENTERED    MN       ENTERED    SIN4/3   ENTERED
 C2N2     ENTERED    C60      ENTERED    MO       ENTERED    VA       ENTERED
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 t
Min value /0/: 200
Max value /1/: 1000
Increment /20/: 10
POLY_3:
POLY_3: save tcex44 y
POLY_3: @@ Step in temperature in order to evaluate proof strength
POLY_3: @@ as function of temperature.
POLY_3: step normal
 No initial equilibrium, using default
 Step will start from axis value    500.000
 POLY has calculated initial equilibrium

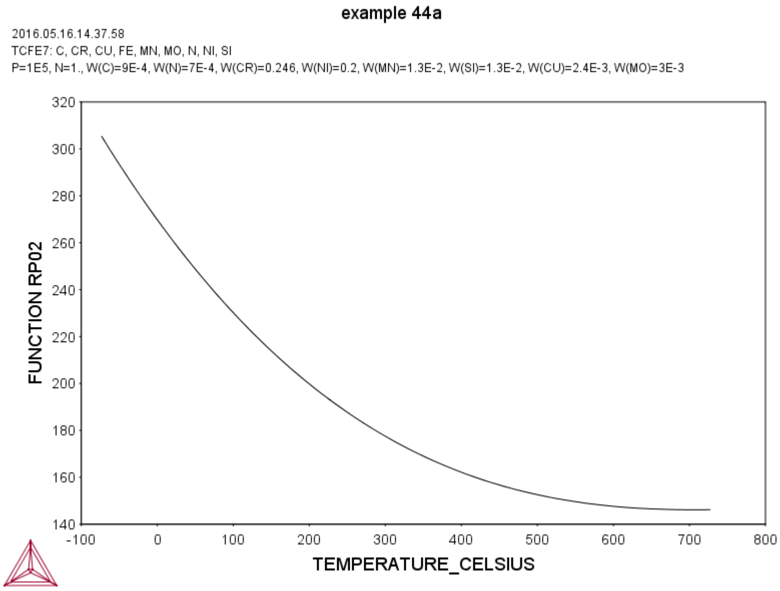
 Phase Region from    500.000     for:
     FCC_A1
 Terminating at   1000.000
 Calculated    53 equilibria

 Phase Region from    500.000     for:
     FCC_A1
 Terminating at    200.000
 Calculated    33 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex44\tcex
 44.POLY3
POLY_3: post

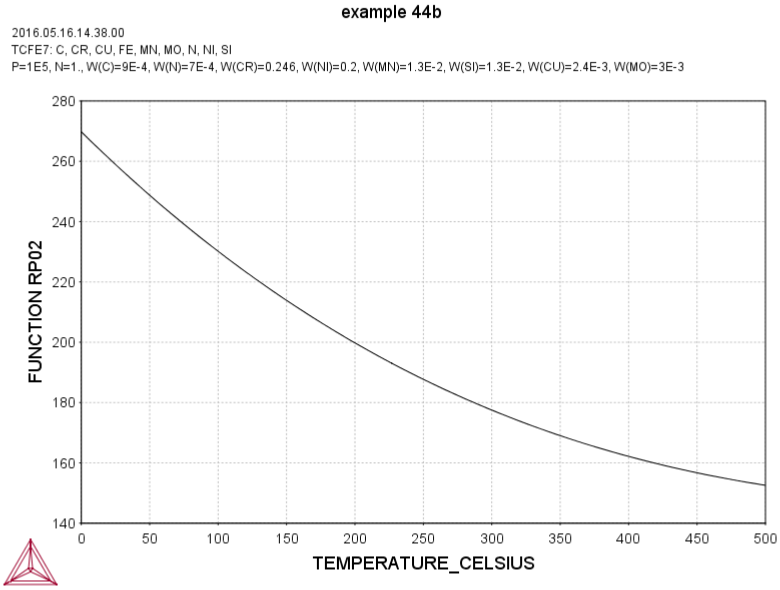
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

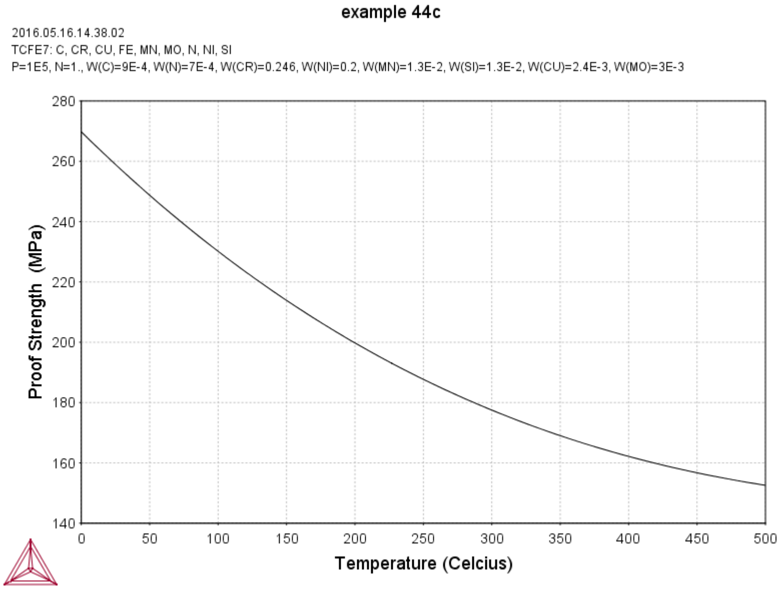
POST: s-d-a y rp02
POST: s-d-a x t-c
POST:
POST: set-title example 44a
POST: plot
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: s-s-s x n 0 500
POST:
POST: set-ras y
POST:
POST: set-title example 44b
POST:
POST: plot
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: set-axis-text-status
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT  (Y OR N) /N/: n
AXIS TEXT : Proof Strength  (MPa)
POST:
POST: set-axis-text-status
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT  (Y OR N) /N/: n
AXIS TEXT : Temperature (Celcius)
POST:
POST: set-title example 44c
POST:
POST: plot
```



```
POST:
POST: set-inter
POST:
```

tcex45

```
About Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\tcex45.TCM" set-echo
SYS: @@
SYS: @@ 3D-Diagram
SYS: @@ with the gamma volume in the Fe-Cr-C system
SYS: @@
SYS: @@ This file calculates the gamma volume in the fe-cr-c system.
SYS: @@ Please note that in order to view the generated file, tcex45.wrl,
SYS: @@ it's necessary to install a WRML(Wirtual Reality Modelling
SYS: @@ Language) viewer to the web browser in use. WRML viwers can be
SYS: @@ downloaded from e.g. www.parallelgraphics.com and www.sim.no
SYS:
SYS: set-log  ex45,,,
SYS:
SYS: @@ Start with calculating the Fe-C side of the diagram
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw FEDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys fe c
   ... the command in full is DEFINE_SYSTEM
 FE                      C  DEFINED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1963 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 800 1800 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3:
POLY_3: save tcex45 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
```

```
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
 Generating start point  31
 Generating start point  32

 Phase region boundary   1 at:   5.236E-01  1.137E+03
     FCC_A1
  ** GRAPHITE
 Calculated.                     14  equilibria

 Phase region boundary   2 at:   5.155E-01  1.011E+03
  ** BCC_A2
     FCC_A1
  ** GRAPHITE

 Phase region boundary   3 at:   1.587E-02  1.011E+03
  ** BCC_A2
     FCC_A1
 Calculated                     38  equilibria

 Phase region boundary   4 at:   5.155E-01  1.011E+03
     FCC_A1
  ** GRAPHITE
 Calculated.                     43  equilibria

 Phase region boundary   5 at:   5.439E-01  1.427E+03
  ** LIQUID
     FCC_A1
  ** GRAPHITE

 Phase region boundary   6 at:   1.310E-01  1.427E+03
  ** LIQUID
     FCC_A1
 Calculated.                     36  equilibria

 Phase region boundary   7 at:   1.599E-02  1.768E+03
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary   8 at:   6.113E-03  1.768E+03
  ** BCC_A2
     FCC_A1
 Calculated                     26  equilibria

 Phase region boundary   9 at:   5.236E-01  1.137E+03
     FCC_A1
  ** GRAPHITE
 Calculated.                     30  equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   5.236E-01  1.137E+03
     FCC_A1
  ** GRAPHITE
 Calculated.                     14  equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   5.236E-01  1.137E+03
     FCC_A1
  ** GRAPHITE
 Calculated.                     30  equilibria
 Terminating at known equilibrium

 Phase region boundary  12 at:   1.216E-01  1.463E+03
  ** LIQUID
     FCC_A1
 Calculated.                      5  equilibria
 Terminating at known equilibrium

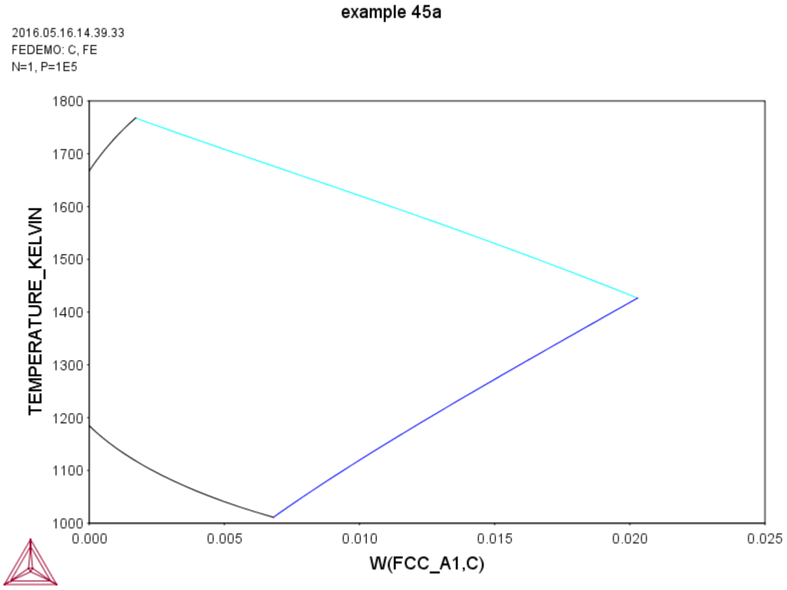
 Phase region boundary  13 at:   1.216E-01  1.463E+03
  ** LIQUID
     FCC_A1
 Calculated.                     32  equilibria
 Terminating at known equilibrium
```

```
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\tcex
 45.POLY3
 CPU time for mapping                       1  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x w(fcc_a1,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the fcc_a1 phase, in the second Cr content which is "zero"
POST: @@ here, and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(fcc_a1,c),zero,T
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fec.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Next step is to calculate the Fe-Cr side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
   ... the command in full is REJECT
 VA                        /-  DEFINED
 REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr
   ... the command in full is DEFINE_SYSTEM
 FE                        CR  DEFINED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
      (1986); CR-FE-MO'
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, estimated parameter 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
```

```
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          6005 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 800 1800 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3:
POLY_3: save tcex45 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Working hard
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   1.067E-02  1.169E+03
     BCC_A2
  ** FCC_A1
 Calculated                     11  equilibria

 Phase region boundary   2 at:   1.067E-02  1.169E+03
     BCC_A2
  ** FCC_A1
 Calculated                     92  equilibria

 Phase region boundary   3 at:   4.325E-02  1.137E+03
     BCC_A2
  ** FCC_A1
 Calculated                     83  equilibria

 Phase region boundary   4 at:   4.325E-02  1.137E+03
     BCC_A2
  ** FCC_A1
 Calculated                     16  equilibria

 Phase region boundary   5 at:   1.006E-01  1.137E+03
     BCC_A2
  ** FCC_A1
 Calculated                     32  equilibria

 Phase region boundary   6 at:   1.006E-01  1.137E+03
     BCC_A2
  ** FCC_A1
 Calculated                     75  equilibria

 Phase region boundary   7 at:   1.051E-01  1.463E+03
```

```
  ** BCC_A2
     FCC_A1
 Calculated                     63  equilibria

 Phase region boundary   8 at:   1.051E-01  1.463E+03
  ** BCC_A2
     FCC_A1
 Calculated                     38  equilibria

 Phase region boundary   9 at:   1.051E-01  1.463E+03
     BCC_A2
  ** FCC_A1
 Calculated                     63  equilibria

 Phase region boundary  10 at:   1.051E-01  1.463E+03
     BCC_A2
  ** FCC_A1
 Calculated                     38  equilibria

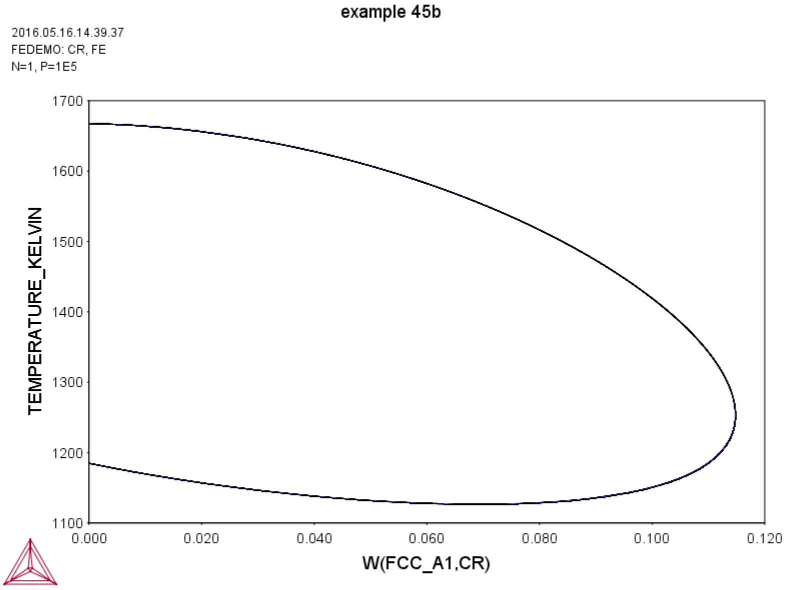
 Phase region boundary  11 at:   9.912E-03  1.665E+03
     BCC_A2
  ** FCC_A1
 Calculated                     15  equilibria

 Phase region boundary  12 at:   9.912E-03  1.665E+03
     BCC_A2
  ** FCC_A1
 Calculated                     88  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\tcex
 45.POLY3
 CPU time for mapping                     2  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x W(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the fcc_a1 phase, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): zero,W(fcc_a1,cr),T
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fecr.tab
   ... the command in full is TABULATE
POST:
POST: @@ Now let's calculate the ternary projection of the fcc_a1 phase
POST: back
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
   ... the command in full is REJECT
 VA                      /-  DEFINED
 REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
   DEFINED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
```

```
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
      (1986); CR-FE-MO'
  'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, estimated parameter 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: se-con t=1050
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1100
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1200
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1300
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
```

```
POLY_3:
POLY_3: se-con t=1400
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1500
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1600
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1700
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3:
POLY_3: save fecrc y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17

 Phase region boundary   1 at:   1.591E-01  2.037E-01
     FCC_A1
  ** M7C3
 Calculated.                       5  equilibria

 Phase region boundary   2 at:   1.629E-01  1.729E-01
  ** CEMENTITE
     FCC_A1
  ** M7C3

 Phase region boundary   3 at:   1.379E-01  8.893E-02
  ** CEMENTITE
     FCC_A1
 Calculated.                       8  equilibria

 Phase region boundary   4 at:   1.434E-01  1.958E-02
  ** CEMENTITE
     FCC_A1
  ** GRAPHITE

 Phase region boundary   5 at:   5.184E-01  1.508E-03
     FCC_A1
  ** GRAPHITE
 Calculated                       9  equilibria

 Phase region boundary   6 at:   1.629E-01  1.729E-01
     FCC_A1
  ** M7C3
 Calculated.                       5  equilibria

 Phase region boundary   7 at:   1.591E-01  2.037E-01
  ** BCC_A2
     FCC_A1
  ** M7C3

 Phase region boundary   8 at:   9.381E-03  1.618E-02
```

```
 ** BCC_A2
    FCC_A1
Calculated                     12  equilibria

Phase region boundary   9 at:   9.381E-03  1.618E-02
    BCC_A2
 ** FCC_A1
Calculated                     14  equilibria

Phase region boundary  10 at:   1.633E-01  1.837E-01
    FCC_A1
 ** M7C3
Calculated.                      3  equilibria

Phase region boundary  11 at:   1.652E-01  1.705E-01
 ** CEMENTITE
    FCC_A1
 ** M7C3

Phase region boundary  12 at:   1.402E-01  9.104E-02
 ** CEMENTITE
    FCC_A1
Calculated.                      9  equilibria

Phase region boundary  13 at:   1.466E-01  1.470E-02
 ** CEMENTITE
    FCC_A1
 ** GRAPHITE

Phase region boundary  14 at:   5.216E-01  1.359E-03
    FCC_A1
 ** GRAPHITE
Calculated                     11  equilibria

Phase region boundary  15 at:   1.652E-01  1.705E-01
    FCC_A1
 ** M7C3
Calculated.                     19  equilibria

Phase region boundary  16 at:   1.521E-01  3.433E-01
    FCC_A1
 ** M23C6
 ** M7C3

Phase region boundary  17 at:   1.055E-01  3.150E-01
    FCC_A1
 ** M23C6
Calculated.                      2  equilibria

Phase region boundary  18 at:   1.054E-01  3.213E-01
 ** BCC_A2
    FCC_A1
 ** M23C6

Phase region boundary  19 at:   2.070E-03  1.073E-01
 ** BCC_A2
    FCC_A1
Calculated                     23  equilibria

Phase region boundary  20 at:   1.633E-01  1.837E-01
    FCC_A1
 ** M7C3
Calculated.                     17  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   1.472E-01  7.619E-02
 ** CEMENTITE
    FCC_A1
Calculated.                      8  equilibria

Phase region boundary  22 at:   1.534E-01  7.611E-03
 ** CEMENTITE
    FCC_A1
 ** GRAPHITE

Phase region boundary  23 at:   5.284E-01  9.641E-04
    FCC_A1
 ** GRAPHITE
Calculated                     11  equilibria

Phase region boundary  24 at:   1.534E-01  7.611E-03
 ** CEMENTITE
    FCC_A1
Calculated.                     10  equilibria

Phase region boundary  25 at:   1.456E-01  9.385E-02
 ** CEMENTITE
    FCC_A1
 ** M7C3

Phase region boundary  26 at:   1.706E-01  1.651E-01
    FCC_A1
 ** M7C3
Calculated.                     20  equilibria

Phase region boundary  27 at:   1.540E-01  3.475E-01
    FCC_A1
 ** M23C6
 ** M7C3

Phase region boundary  28 at:   1.074E-01  3.204E-01
    FCC_A1
 ** M23C6
Calculated.                      5  equilibria

Phase region boundary  29 at:   1.065E-01  3.518E-01
 ** BCC_A2
    FCC_A1
 ** M23C6

Phase region boundary  30 at:   3.537E-03  1.631E-01
 ** BCC_A2
    FCC_A1
Calculated                     17  equilibria

Phase region boundary  31 at:   1.472E-01  7.619E-02
```

```
 ** CEMENTITE
    FCC_A1
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   1.555E-01  5.938E-02
 ** CEMENTITE
    FCC_A1
Calculated.                      8  equilibria

Phase region boundary  33 at:   1.603E-01  4.094E-03
 ** CEMENTITE
    FCC_A1
 ** GRAPHITE

Phase region boundary  34 at:   5.353E-01  6.720E-04
    FCC_A1
 ** GRAPHITE
Calculated                     11  equilibria

Phase region boundary  35 at:   1.603E-01  4.094E-03
 ** CEMENTITE
    FCC_A1
Calculated.                     11  equilibria

Phase region boundary  36 at:   1.523E-01  9.416E-02
 ** CEMENTITE
    FCC_A1
 ** M7C3

Phase region boundary  37 at:   1.773E-01  1.579E-01
    FCC_A1
 ** M7C3
Calculated.                     21  equilibria

Phase region boundary  38 at:   1.566E-01  3.575E-01
    FCC_A1
 ** M23C6
 ** M7C3

Phase region boundary  39 at:   1.100E-01  3.333E-01
    FCC_A1
 ** M23C6
Calculated.                      3  equilibria

Phase region boundary  40 at:   1.093E-01  3.506E-01
 ** BCC_A2
    FCC_A1
 ** M23C6

Phase region boundary  41 at:   6.971E-03  1.843E-01
 ** BCC_A2
    FCC_A1
Calculated                     15  equilibria

Phase region boundary  42 at:   1.555E-01  5.938E-02
 ** CEMENTITE
    FCC_A1
Calculated.                      5  equilibria
Terminating at known equilibrium

Phase region boundary  43 at:   1.641E-01  4.814E-02
 ** CEMENTITE
    FCC_A1
Calculated.                      6  equilibria

Phase region boundary  44 at:   1.675E-01  4.450E-03
 ** CEMENTITE
    FCC_A1
 ** GRAPHITE

Phase region boundary  45 at:   5.425E-01  9.066E-04
    FCC_A1
 ** GRAPHITE
Calculated                     12  equilibria

Phase region boundary  46 at:   1.675E-01  4.450E-03
 ** CEMENTITE
    FCC_A1
Calculated.                     10  equilibria

Phase region boundary  47 at:   1.603E-01  9.101E-02
 ** CEMENTITE
    FCC_A1
 ** M7C3

Phase region boundary  48 at:   1.853E-01  1.474E-01
    FCC_A1
 ** M7C3
Calculated.                     24  equilibria

Phase region boundary  49 at:   1.599E-01  3.696E-01
 ** BCC_A2
    FCC_A1
 ** M7C3

Phase region boundary  50 at:   1.213E-02  2.017E-01
 ** BCC_A2
    FCC_A1
Calculated                     26  equilibria

Phase region boundary  51 at:   1.641E-01  4.814E-02
 ** CEMENTITE
    FCC_A1
Calculated.                      6  equilibria
Terminating at known equilibrium

Phase region boundary  52 at:   1.142E-01  2.495E-02
 ** LIQUID
    FCC_A1
Calculated                     16  equilibria

Phase region boundary  53 at:   1.142E-01  2.495E-02
 ** LIQUID
    FCC_A1
Calculated.                      6  equilibria
```

```
 Phase region boundary  54 at:   1.177E-01  7.477E-02
  ** LIQUID
     FCC_A1
  ** M7C3

 Phase region boundary  55 at:   1.877E-01  1.707E-01
     FCC_A1
  ** M7C3
 Calculated.                      21  equilibria

 Phase region boundary  56 at:   1.645E-01  3.686E-01
  ** BCC_A2
     FCC_A1
  ** M7C3

 Phase region boundary  57 at:   1.810E-02  2.160E-01
  ** BCC_A2
     FCC_A1
 Calculated                      20  equilibria

 Phase region boundary  58 at:   1.177E-01  7.477E-02
  ** LIQUID
     FCC_A1
 Calculated                      21  equilibria

 Phase region boundary  59 at:   8.271E-02  2.328E-02
  ** LIQUID
     FCC_A1
 Calculated                      11  equilibria

 Phase region boundary  60 at:   8.271E-02  2.328E-02
  ** LIQUID
     FCC_A1
 Calculated.                      23  equilibria

 Phase region boundary  61 at:   6.085E-02  2.377E-01
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary  62 at:   2.036E-02  2.062E-01
  ** BCC_A2
     FCC_A1
 Calculated                      30  equilibria

 Phase region boundary  63 at:   6.085E-02  2.377E-01
  ** LIQUID
     FCC_A1
 Calculated                      35  equilibria

 Phase region boundary  64 at:   4.494E-02  2.178E-02
  ** LIQUID
     FCC_A1
 Calculated                      16  equilibria

 Phase region boundary  65 at:   4.494E-02  2.178E-02
  ** LIQUID
     FCC_A1
 Calculated.                      13  equilibria

 Phase region boundary  66 at:   3.129E-02  1.383E-01
  ** LIQUID
  ** BCC_A2
     FCC_A1

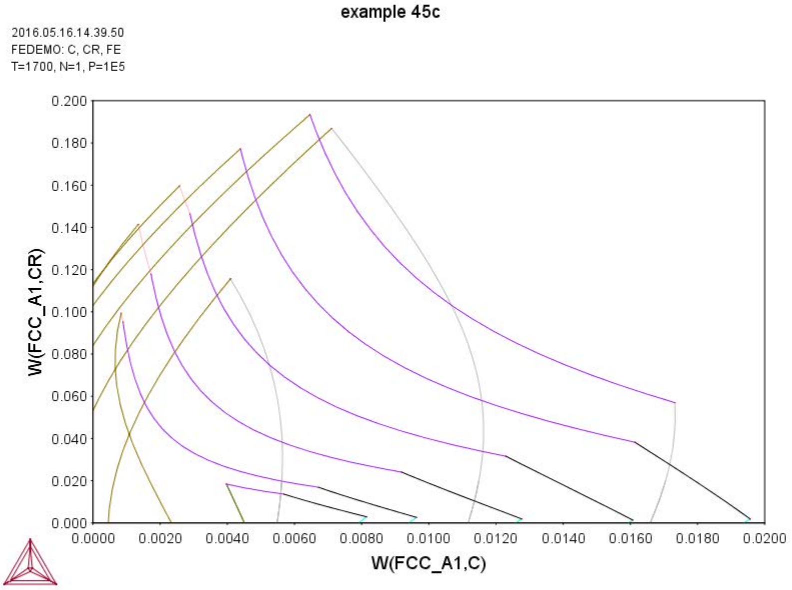
 Phase region boundary  67 at:   1.259E-02  1.273E-01
  ** BCC_A2
     FCC_A1
 Calculated                      25  equilibria

 Phase region boundary  68 at:   3.129E-02  1.383E-01
  ** LIQUID
     FCC_A1
 Calculated                      28  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\fecr
 c.POLY3
 CPU time for mapping                      5  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x W(fcc_a1,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: back
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 3 T 800 2000 5
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: se-con x(cr)=.1
   ... the command in full is SET_CONDITION
POLY_3: se-con x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-con t=1373
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16532 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: ad-ini 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /FCC_A1#1/: fcc_a1
POLY_3:
POLY_3: map
 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18

 Phase region boundary   1 at:    5.770E-04  1.292E-02  1.050E+03
     BCC_A2
  ** FCC_A1
  ** M7C3
 CALCULATED      7 EQUILIBRIA

 Phase region boundary   2 at:    6.909E-04  7.705E-03  1.030E+03
     BCC_A2
     CEMENTITE
  ** FCC_A1
  ** M7C3

 Phase region boundary   2 at:    3.000E-01  3.347E-01  1.030E+03
  ** CEMENTITE
  ** FCC_A1
     M7C3
 CALCULATED     89 EQUILIBRIA

 Phase region boundary   2 at:    8.299E-02  4.133E-02  1.467E+03
     LIQUID
  ** CEMENTITE
     FCC_A1
```

```
 ** M7C3
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary   2 at:   8.299E-02  4.133E-02  1.467E+03
 ** LIQUID
 ** CEMENTITE
    FCC_A1
Terminating at diagram limit
CALCULATED    11 EQUILIBRIA

Phase region boundary   2 at:   8.299E-02  4.133E-02  1.467E+03
 ** LIQUID
    FCC_A1
 ** M7C3
CALCULATED    31 EQUILIBRIA

Phase region boundary   2 at:   3.564E-02  2.106E-01  1.567E+03
 ** LIQUID
    BCC_A2
    FCC_A1
 ** M7C3
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary   2 at:   3.564E-02  2.106E-01  1.567E+03
 ** LIQUID
 ** BCC_A2
    FCC_A1
Terminating at diagram limit
CALCULATED    48 EQUILIBRIA

Phase region boundary   2 at:   3.564E-02  2.106E-01  1.567E+03
 ** BCC_A2
    FCC_A1
 ** M7C3
CALCULATED    40 EQUILIBRIA

Phase region boundary   2 at:   1.817E-02  1.819E-01  1.380E+03
 ** BCC_A2
    FCC_A1
    M23C6
 ** M7C3
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary   2 at:   1.817E-02  1.819E-01  1.380E+03
 ** BCC_A2
    FCC_A1
 ** M23C6
CALCULATED    60 EQUILIBRIA

Phase region boundary   2 at:   3.999E-03  1.003E-01  1.096E+03
 ** BCC_A2
    FCC_A1
 ** M23C6
    M7C3
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary   2 at:   3.999E-03  1.003E-01  1.096E+03
 ** BCC_A2
    FCC_A1
 ** M7C3
Terminating at known equilibrium
CALCULATED    18 EQUILIBRIA

Phase region boundary   2 at:   3.999E-03  1.003E-01  1.096E+03
    FCC_A1
 ** M23C6
 ** M7C3
Terminating at known equilibrium
CALCULATED    60 EQUILIBRIA

Phase region boundary   2 at:   6.909E-04  7.705E-03  1.030E+03
    BCC_A2
 ** CEMENTITE
 ** FCC_A1
CALCULATED     7 EQUILIBRIA

Phase region boundary   2 at:   8.322E-04  1.593E-03  1.008E+03
    BCC_A2
 ** CEMENTITE
 ** FCC_A1
    GRAPHITE

Phase region boundary   2 at:   1.000E+00  0.000E+00  1.008E+03
 ** CEMENTITE
 ** FCC_A1
    GRAPHITE
OUTSIDE AXIS LIMITS
Terminating at diagram limit
CALCULATED     6 EQUILIBRIA
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary   2 at:   8.322E-04  1.593E-03  1.008E+03
    BCC_A2
 ** FCC_A1
 ** GRAPHITE
Terminating at diagram limit
CALCULATED     8 EQUILIBRIA
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary   2 at:   5.770E-04  1.292E-02  1.050E+03
    BCC_A2
 ** FCC_A1
 ** M7C3
Terminating at known equilibrium
CALCULATED    15 EQUILIBRIA

Phase region boundary   2 at:   2.668E-02  2.000E-02  1.051E+03
 ** BCC_A2
    FCC_A1
 ** M7C3
Terminating at known equilibrium
CALCULATED     7 EQUILIBRIA

Phase region boundary   2 at:   2.668E-02  2.000E-02  1.051E+03
 ** BCC_A2
    FCC_A1
```

```
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    14 EQUILIBRIA

 Phase region boundary   2 at:   4.444E-02  2.000E-02  1.133E+03
  ** CEMENTITE
     FCC_A1
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    24 EQUILIBRIA

 Phase region boundary   2 at:   4.444E-02  2.000E-02  1.133E+03
  ** CEMENTITE
     FCC_A1
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    70 EQUILIBRIA

 Phase region boundary   2 at:   6.099E-02  2.000E-02  1.133E+03
  ** CEMENTITE
     FCC_A1
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    24 EQUILIBRIA

 Phase region boundary   2 at:   6.099E-02  2.000E-02  1.133E+03
  ** CEMENTITE
     FCC_A1
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    70 EQUILIBRIA

 Phase region boundary   2 at:   7.812E-02  2.000E-02  1.133E+03
  ** CEMENTITE
     FCC_A1
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    24 EQUILIBRIA

 Phase region boundary   2 at:   7.812E-02  2.000E-02  1.133E+03
  ** CEMENTITE
     FCC_A1
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    70 EQUILIBRIA

 Phase region boundary   2 at:   7.451E-02  2.000E-02  1.446E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA

 Phase region boundary   2 at:   7.451E-02  2.000E-02  1.446E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
 Terminating at known equilibrium
 CALCULATED     7 EQUILIBRIA

 Phase region boundary   2 at:   5.118E-02  2.000E-02  1.446E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA

 Phase region boundary   2 at:   5.118E-02  2.000E-02  1.446E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
 Terminating at known equilibrium
 CALCULATED     7 EQUILIBRIA

 Phase region boundary   2 at:   2.557E-02  2.000E-02  1.446E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA

 Phase region boundary   2 at:   2.557E-02  2.000E-02  1.446E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
 Terminating at known equilibrium
 CALCULATED     7 EQUILIBRIA

 Phase region boundary   2 at:   2.829E-02  1.000E-01  1.096E+03
  ** BCC_A2
     FCC_A1
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    14 EQUILIBRIA

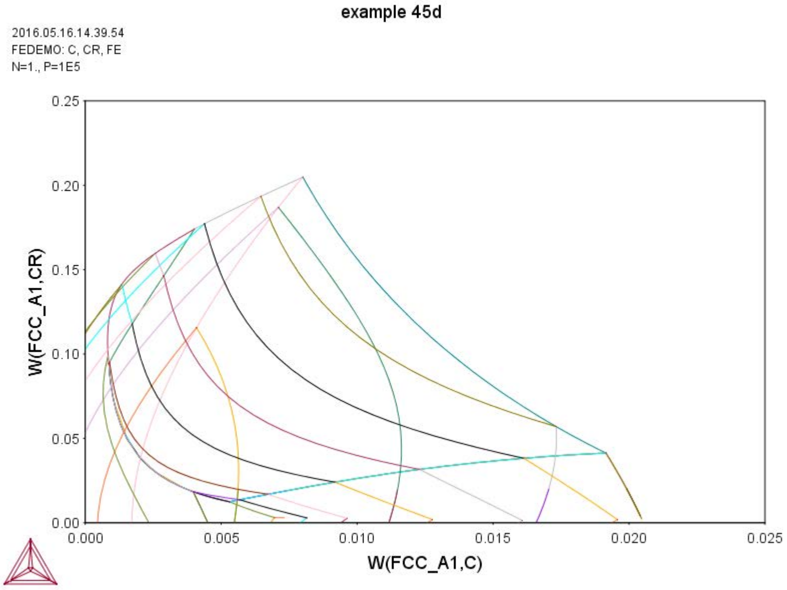
 Phase region boundary   2 at:   2.829E-02  1.000E-01  1.096E+03
  ** BCC_A2
     FCC_A1
  ** M7C3
 Terminating at known equilibrium
 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\fecr
 c.POLY3
 CPU time for mapping                      2  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x W(fcc_a1,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
```

```
POST: set-title example 45d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter the table for the calculated data.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(fcc_a1,c),W(fcc_a1,cr),T;
POST:
POST: tab tab1 fecrc.tab
   ... the command in full is TABULATE
POST:
POST: @@ Set the axis variables and the axis text for the final diagram
POST: s-a-t-s x n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac C
POST: s-a-t-s y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac Cr
POST:
POST: s-d-a z temp-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-t-s z n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Temp C
POST:
POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data
POST: @@ from the different tables created and saved. This is accomplished
POST: @@ using the command "CREATE_3D_DIAGRAM". Also define the scaling
POST: @@ to be used in the 3D-diagram.
POST: cre-3d
   ... the command in full is CREATE_3D_PLOTFILE
Use current WORKSPACE (WS), TAB files or BOTH: /WS/: BOTH
 The table must contain values for X,Y and Z axis
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    TEMP_C=T-273.15
 DEFINED TABLES
    TAB1=W(FCC_A1,C), W(FCC_A1,CR), T
Table Name: tab1
Give TAB filename: /Cancel_to_finish/: fec.tab fecr.tab Cancel_to_finish
Output file: /3Dplot/: tcex45.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/: .02
Y-AXIS SCALING FROM 0.0 TO YMAX /1/: .20
Z-AXIS SCALING, GIVE ZMIN /0/: 1000
Z-AXIS SCALING, GIVE ZMAX /2000/: 2000

 It is possible to combine files by:
 Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

 Processing fec.tab
   3.538090000000000E-010 <X<  2.028510000000000E-002
   0.000000000000000E+000 <Y<  0.000000000000000E+000
    1011.18000000000      <Z<   1767.78000000000

 Processing fecr.tab
   0.000000000000000E+000 <X<  0.000000000000000E+000
   2.741540000000000E-009 <Y<  0.114805000000000
    1126.34000000000      <Z<   1667.47000000000
POST:
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex46

```
About License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\tcex46.TCM"SYS: set-echo
SYS: @@
SYS: @@ 3D-Diagram
SYS: @@ with the liquidus surface of the Fe-Cr-C system
SYS: @@
SYS: @@This file calculates the Liquidus surface in the FE-CR-C system
SYS: @@ Please note that in order to view the generated files, tcex46_tri.wrl
SYS: @@ and tcex46_sqrt, it's necessary to install a WRML(Wirtual Reality
SYS: @@ Modelling Language) viewer to the web browser in use. WRML viwers
SYS: @@ can be downloaded from e.g. www.parallelgraphics.com and
SYS: @@ www.sim.no
SYS:
SYS: set-log ex46,,
SYS:
SYS: @@ Start by calculating the Fe-C side of the diagram
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw tcfe7
   ... the command in full is SWITCH_DATABASE
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE7: de-sys fe c
   ... the command in full is DEFINE_SYSTEM
 FE                      C  DEFINED
TDB_TCFE7: rej-ph * all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M5C2                    KSI_CARBIDE
 A1_KAPPA                KAPPA                   FE4N_LP1
 FECN_CHI                LAVES_PHASE_C14  REJECTED
TDB_TCFE7: res-ph fcc_a1,bcc_a2,cementite,graphite,liquid
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  CEMENTITE
 GRAPHITE                LIQUID:L  RESTORED
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 -OK-
TDB_TCFE7:
TDB_TCFE7: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1973
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           413 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1300 5000 20
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liq
POLY_3:
POLY_3: save tcex46 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
```

```
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   1.982E-02  1.759E+03
  ** LIQUID
     FCC_A1
 Calculated.                       2  equilibria

 Phase region boundary   2 at:   1.599E-02  1.768E+03
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary   3 at:   1.417E-02  1.768E+03
     LIQUID
  ** BCC_A2
 Calculated                      15  equilibria

 Phase region boundary   4 at:   1.599E-02  1.768E+03
  ** LIQUID
     FCC_A1
 Calculated.                      19  equilibria

 Phase region boundary   5 at:   1.310E-01  1.427E+03
  ** LIQUID
     FCC_A1
  ** GRAPHITE

 Phase region boundary   6 at:   5.871E-01  1.427E+03
     LIQUID
  ** GRAPHITE
 Calculated                     178  equilibria

 Phase region boundary   7 at:   1.982E-02  1.759E+03
  ** LIQUID
     FCC_A1
 Calculated.                      24  equilibria
 Terminating at known equilibrium

 Phase region boundary   8 at:   6.344E-01  2.537E+03
     LIQUID
  ** GRAPHITE
 Calculated.                      57  equilibria
 Terminating at known equilibrium

 Phase region boundary   9 at:   6.344E-01  2.537E+03
     LIQUID
  ** GRAPHITE
 Calculated                     128  equilibria

 Phase region boundary  10 at:   6.344E-01  2.537E+03
     LIQUID
  ** GRAPHITE
 Calculated.                      57  equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   6.344E-01  2.537E+03
     LIQUID
  ** GRAPHITE
 Calculated                     128  equilibria

 Phase region boundary  12 at:   7.226E-01  3.763E+03
     LIQUID
  ** GRAPHITE
 Calculated.                     118  equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   7.226E-01  3.763E+03
     LIQUID
  ** GRAPHITE
 Calculated                      64  equilibria

 Phase region boundary  14 at:   7.226E-01  3.763E+03
     LIQUID
  ** GRAPHITE
 Calculated.                     118  equilibria
 Terminating at known equilibrium

 Phase region boundary  15 at:   7.226E-01  3.763E+03
     LIQUID
```

```
  ** GRAPHITE
 Calculated                      64  equilibria

 Phase region boundary  16 at:   5.888E-03  1.794E+03
     LIQUID
  ** BCC_A2
 Calculated                      13  equilibria

 Phase region boundary  17 at:   5.888E-03  1.794E+03
     LIQUID
  ** BCC_A2
 Calculated.                       3  equilibria
 Terminating at known equilibrium

 Phase region boundary  18 at:   6.683E-01  3.181E+03
     LIQUID
  ** GRAPHITE
 Calculated.                      89  equilibria
 Terminating at known equilibrium

 Phase region boundary  19 at:   6.683E-01  3.181E+03
     LIQUID
  ** GRAPHITE
 Calculated                      92  equilibria

 Phase region boundary  20 at:   8.317E-01  4.174E+03
     LIQUID
  ** GRAPHITE
 Calculated.                     147  equilibria
 Terminating at known equilibrium

 Phase region boundary  21 at:   8.317E-01  4.174E+03
     LIQUID
  ** GRAPHITE
 Calculated                      43  equilibria

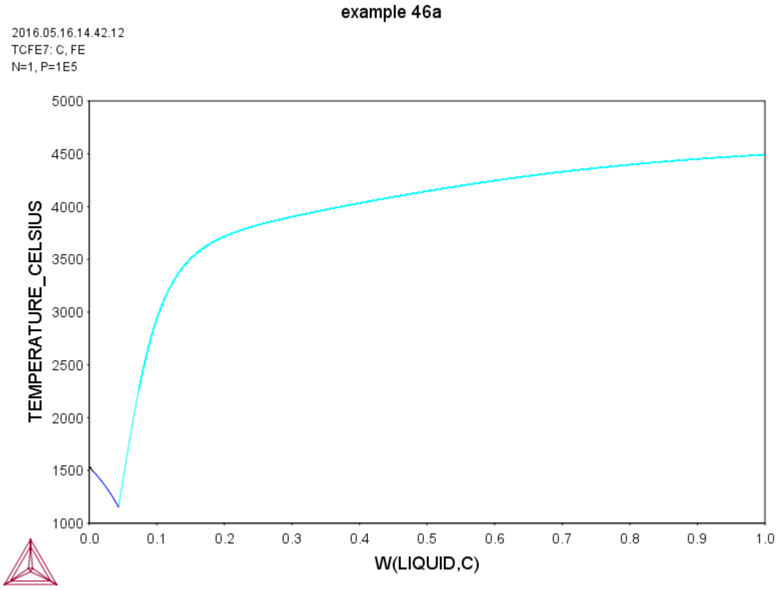
 Phase region boundary  22 at:   9.950E-01  4.749E+03
     LIQUID
  ** GRAPHITE
 Calculated.                     179  equilibria
 Terminating at known equilibrium

 Phase region boundary  23 at:   9.950E-01  4.749E+03
     LIQUID
  ** GRAPHITE
 Calculated                      18  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\tcex
 46.POLY3
 CPU time for mapping                      1   seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x w(liquid,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tabl
   ... the command in full is ENTER_SYMBOL
Variable(s): W(liquid,c),zero,Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tabl fec_liq.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Next calculate the Fe-Cr side of the diagram
```

```
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE7: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
TDB_TCFE7: de-sys fe cr
   ... the command in full is DEFINE_SYSTEM
 FE                      CR  DEFINED
TDB_TCFE7: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  A1_KAPPA                KAPPA
 SIGMA                   CHI_A12                 LAVES_PHASE_C14
 CR3SI  REJECTED
TDB_TCFE7: res-ph bcc_a2,liquid
   ... the command in full is RESTORE
 BCC_A2                  LIQUID:L  RESTORED
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
 -OK-
TDB_TCFE7:
TDB_TCFE7: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=2373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           274 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1500 2400 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liquid
POLY_3:
POLY_3: save tcex46 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
```

```
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24

Phase region boundary   1 at:   1.039E-02  1.809E+03
 ** LIQUID
    BCC_A2
Calculated                     14  equilibria

Phase region boundary   2 at:   1.039E-02  1.809E+03
 ** LIQUID
    BCC_A2
Calculated                    110  equilibria

Phase region boundary   3 at:   3.280E-01  1.802E+03
 ** LIQUID
    BCC_A2
Calculated                     43  equilibria

Phase region boundary   4 at:   3.280E-01  1.802E+03
 ** LIQUID
    BCC_A2
Calculated                     81  equilibria

Phase region boundary   5 at:   6.371E-01  1.971E+03
 ** LIQUID
    BCC_A2
Calculated                     76  equilibria

Phase region boundary   6 at:   6.371E-01  1.971E+03
 ** LIQUID
    BCC_A2
Calculated                     48  equilibria

Phase region boundary   7 at:   9.888E-01  2.175E+03
 ** LIQUID
    BCC_A2
Calculated                    114  equilibria

Phase region boundary   8 at:   9.888E-01  2.175E+03
 ** LIQUID
    BCC_A2
Calculated                     10  equilibria

Phase region boundary   9 at:   5.100E-02  1.803E+03
 ** LIQUID
    BCC_A2
Calculated                    105  equilibria

Phase region boundary  10 at:   5.100E-02  1.803E+03
 ** LIQUID
    BCC_A2
Calculated                     12  equilibria

Phase region boundary  11 at:   3.337E-01  1.803E+03
 ** LIQUID
    BCC_A2
Calculated                     44  equilibria

Phase region boundary  12 at:   3.337E-01  1.803E+03
 ** LIQUID
    BCC_A2
Calculated                    102  equilibria

Phase region boundary  13 at:   8.293E-01  2.097E+03
    LIQUID
 ** BCC_A2
Calculated                    111  equilibria

Phase region boundary  14 at:   8.293E-01  2.097E+03
    LIQUID
 ** BCC_A2
Calculated                     32  equilibria

Phase region boundary  15 at:   8.293E-01  2.097E+03
 ** LIQUID
    BCC_A2
Calculated                    111  equilibria

Phase region boundary  16 at:   8.293E-01  2.097E+03
 ** LIQUID
    BCC_A2
Calculated                     32  equilibria

Phase region boundary  17 at:   9.640E-03  1.809E+03
    LIQUID
 ** BCC_A2
Calculated                     15  equilibria

Phase region boundary  18 at:   9.640E-03  1.809E+03
    LIQUID
 ** BCC_A2
Calculated                    109  equilibria

Phase region boundary  19 at:   3.471E-01  1.807E+03
    LIQUID
 ** BCC_A2
Calculated                     49  equilibria

Phase region boundary  20 at:   3.471E-01  1.807E+03
    LIQUID
 ** BCC_A2
Calculated                     75  equilibria

Phase region boundary  21 at:   6.881E-01  2.007E+03
    LIQUID
 ** BCC_A2
Calculated                     83  equilibria

Phase region boundary  22 at:   6.881E-01  2.007E+03
    LIQUID
 ** BCC_A2
Calculated                     41  equilibria
```

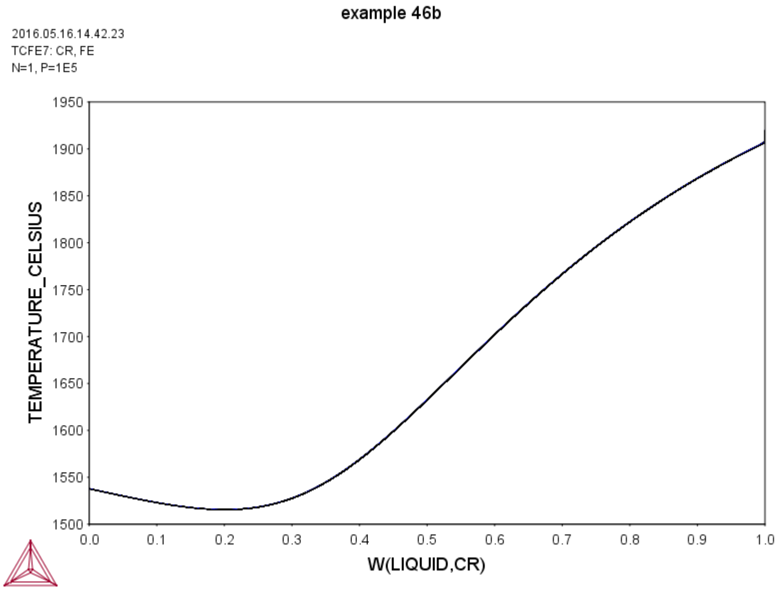
```
 Phase region boundary  23 at:   9.910E-01  2.176E+03
     LIQUID
  ** BCC_A2
 Calculated                    106  equilibria

 Phase region boundary  24 at:   9.910E-01  2.176E+03
     LIQUID
  ** BCC_A2
 Calculated                     14  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\tcex
 46.POLY3
 CPU time for mapping                     1  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x W(liquid,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): zero,W(liquid,cr),Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fecr_liq.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Then calculate the Cr-C side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE7: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
TDB_TCFE7: de-sys c cr
   ... the command in full is DEFINE_SYSTEM
 C                        CR  DEFINED
TDB_TCFE7: rej-ph * all
   ... the command in full is REJECT
 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M3C2                     KSI_CARBIDE
 FE4N_LP1                 SIGMA                    CHI_A12
 LAVES_PHASE_C14          CR3SI  REJECTED
TDB_TCFE7: res-ph bcc_a2,liquid,graphite,m23,m7c,m3c2
   ... the command in full is RESTORE
 BCC_A2                   LIQUID:L                 GRAPHITE
 M23C6                    M7C3                     M3C2
   RESTORED
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data
```

```
  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=2373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=1.5e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           278 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1500 5000 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liq
POLY_3:
POLY_3: save tcex46 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   2.762E-01  2.670E+03
     LIQUID
  ** GRAPHITE
 Calculated.                     61  equilibria

 Phase region boundary   2 at:   3.108E-01  2.077E+03
     LIQUID
  ** GRAPHITE
  ** M3C2

 Phase region boundary   3 at:   6.108E-01  2.077E+03
     LIQUID
  ** M3C2
 Calculated.                      7  equilibria

 Phase region boundary   4 at:   6.354E-01  2.018E+03
     LIQUID
  ** M3C2
```

```
 ** M7C3

Phase region boundary   5 at:   6.854E-01  2.018E+03
    LIQUID
 ** M7C3
Calculated.                      36  equilibria

Phase region boundary   6 at:   7.604E-01  1.850E+03
    LIQUID
 ** M23C6
 ** M7C3

Phase region boundary   7 at:   8.070E-01  1.850E+03
    LIQUID
 ** M23C6
Calculated.                       6  equilibria

Phase region boundary   8 at:   8.281E-01  1.806E+03
    LIQUID
 ** BCC_A2
 ** M23C6

Phase region boundary   9 at:   9.300E-01  1.806E+03
    LIQUID
 ** BCC_A2
Calculated                      54  equilibria

Phase region boundary  10 at:   3.108E-01  2.077E+03
    LIQUID
 ** GRAPHITE
Calculated                     289  equilibria

Phase region boundary  11 at:   2.762E-01  2.670E+03
    LIQUID
 ** GRAPHITE
Calculated                     222  equilibria

Phase region boundary  12 at:   2.762E-01  2.670E+03
    LIQUID
 ** GRAPHITE
Calculated.                      61  equilibria
Terminating at known equilibrium

Phase region boundary  13 at:   2.762E-01  2.670E+03
    LIQUID
 ** GRAPHITE
Calculated                     222  equilibria

Phase region boundary  14 at:   2.023E-01  3.830E+03
    LIQUID
 ** GRAPHITE
Calculated.                     177  equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   2.023E-01  3.830E+03
    LIQUID
 ** GRAPHITE
Calculated                     106  equilibria

Phase region boundary  16 at:   2.023E-01  3.830E+03
    LIQUID
 ** GRAPHITE
Calculated.                     177  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   2.023E-01  3.830E+03
    LIQUID
 ** GRAPHITE
Calculated                     106  equilibria

Phase region boundary  18 at:   5.000E-03  4.751E+03
    LIQUID
 ** GRAPHITE
Calculated                      18  equilibria

Phase region boundary  19 at:   5.000E-03  4.751E+03
    LIQUID
 ** GRAPHITE
Calculated.                     276  equilibria
Terminating at known equilibrium

Phase region boundary  20 at:   1.683E-01  4.226E+03
    LIQUID
 ** GRAPHITE
Calculated                      73  equilibria

Phase region boundary  21 at:   1.683E-01  4.226E+03
    LIQUID
 ** GRAPHITE
Calculated.                     216  equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   6.317E-01  2.031E+03
    LIQUID
 ** M3C2
Calculated.                       7  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   6.317E-01  2.031E+03
    LIQUID
 ** M3C2
Calculated.                       3  equilibria
Terminating at known equilibrium

Phase region boundary  24 at:   9.949E-01  2.162E+03
    LIQUID
 ** BCC_A2
Calculated.                      38  equilibria
Terminating at known equilibrium

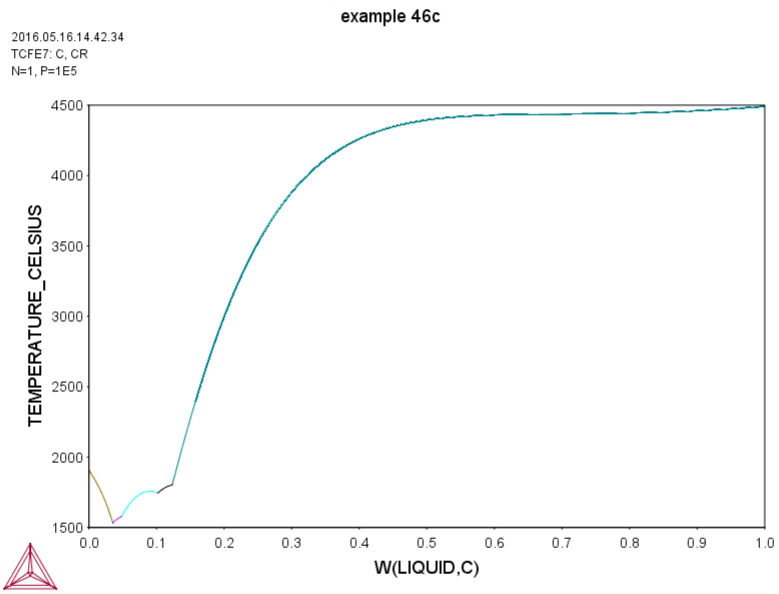
Phase region boundary  25 at:   9.949E-01  2.162E+03
    LIQUID
 ** BCC_A2
Calculated                      14  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\tcex
```

```
 46.POLY3
 CPU time for mapping                     1  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x w(liquid,C)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y temp-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(liquid,c),W(liquid,cr),Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tab1 crc_liq.tab
   ... the command in full is TABULATE
POST:
POST: back
POLY_3: @@ Finnaly, calculate a ternary projection of the Fe-Cr-C system
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE7: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
TDB_TCFE7: de-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
   DEFINED
TDB_TCFE7: rej-ph * all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M5C2                    M3C2
 KSI_CARBIDE             A1_KAPPA                KAPPA
 FE4N_LP1                FECN_CHI                SIGMA
 CHI_A12                 LAVES_PHASE_C14         CR3SI
   REJECTED
TDB_TCFE7: res-ph liquid,fcc_a1,bcc_a2,m23,m7c,m3c2,graphite,cementite
   ... the command in full is RESTORE
 LIQUID:L                FCC_A1                  BCC_A2
 M23C6                   M7C3                    M3C2
 GRAPHITE                CEMENTITE  RESTORED
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

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      -FE'
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      hard mater, Vol. 12, pp. 121-127; Molar volumes'
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  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
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  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
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  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
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 -OK-
TDB_TCFE7:
TDB_TCFE7: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: se-con t=1600
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1700
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1800
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2100
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2200
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
```

```
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=9e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: se-con t=1900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2100
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liq
POLY_3:
POLY_3: save fecrc y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard

 Phase region boundary   1 at:   8.271E-02  2.328E-02
  ** LIQUID
     FCC_A1
 Calculated                     11  equilibria

 Phase region boundary   2 at:   8.271E-02  2.328E-02
  ** LIQUID
     FCC_A1
 Calculated.                     23  equilibria

 Phase region boundary   3 at:   6.085E-02  2.377E-01
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary   4 at:   4.944E-02  2.509E-01
     LIQUID
  ** BCC_A2
 Calculated.                     22  equilibria

 Phase region boundary   5 at:   5.504E-02  4.549E-01
     LIQUID
  ** BCC_A2
  ** M23C6

 Phase region boundary   6 at:   1.550E-01  5.383E-01
     LIQUID
  ** M23C6
 Calculated.                      3  equilibria
```

```
Phase region boundary   7 at:   1.594E-01  5.202E-01
    LIQUID
 ** M23C6
 ** M7C3

Phase region boundary   8 at:   2.060E-01  5.178E-01
    LIQUID
 ** M7C3
Calculated.                      38  equilibria

Phase region boundary   9 at:   2.657E-01  1.556E-01
    LIQUID
 ** GRAPHITE
 ** M7C3

Phase region boundary  10 at:   6.157E-01  4.922E-02
    LIQUID
 ** GRAPHITE
Calculated                     18  equilibria

Phase region boundary  11 at:   6.085E-02  2.377E-01
 ** LIQUID
    FCC_A1
Calculated                     35  equilibria

Phase region boundary  12 at:   4.494E-02  2.178E-02
 ** LIQUID
    FCC_A1
Calculated                     16  equilibria

Phase region boundary  13 at:   4.494E-02  2.178E-02
 ** LIQUID
    FCC_A1
Calculated.                      13  equilibria

Phase region boundary  14 at:   3.129E-02  1.383E-01
 ** LIQUID
 ** BCC_A2
    FCC_A1

Phase region boundary  15 at:   2.528E-02  1.443E-01
    LIQUID
 ** BCC_A2
Calculated.                      59  equilibria

Phase region boundary  16 at:   6.178E-02  7.198E-01
    LIQUID
 ** BCC_A2
 ** M23C6

Phase region boundary  17 at:   1.633E-01  7.006E-01
    LIQUID
 ** M23C6
Calculated.                       7  equilibria

Phase region boundary  18 at:   1.771E-01  6.455E-01
    LIQUID
 ** M23C6
 ** M7C3

Phase region boundary  19 at:   2.237E-01  6.202E-01
    LIQUID
 ** M7C3
Calculated.                      40  equilibria

Phase region boundary  20 at:   2.886E-01  2.325E-01
    LIQUID
 ** GRAPHITE
 ** M7C3

Phase region boundary  21 at:   6.386E-01  9.541E-02
    LIQUID
 ** GRAPHITE
Calculated                     29  equilibria

Phase region boundary  22 at:   3.129E-02  1.383E-01
 ** LIQUID
    FCC_A1
Calculated                     28  equilibria

Phase region boundary  23 at:   6.080E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated                     22  equilibria

Phase region boundary  24 at:   6.080E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated.                      30  equilibria

Phase region boundary  25 at:   6.645E-01  1.791E-01
    LIQUID
 ** GRAPHITE
 ** M7C3

Phase region boundary  26 at:   3.145E-01  3.964E-01
    LIQUID
 ** M7C3
Calculated.                      53  equilibria

Phase region boundary  27 at:   2.351E-01  7.127E-01
    LIQUID
 ** M23C6
 ** M7C3

Phase region boundary  28 at:   1.885E-01  7.542E-01
    LIQUID
 ** M23C6
Calculated.                       8  equilibria

Phase region boundary  29 at:   1.714E-01  8.208E-01
    LIQUID
 ** BCC_A2
 ** M23C6
```

```
Phase region boundary  30 at:   6.952E-02  9.185E-01
    LIQUID
 ** BCC_A2
Calculated                     80  equilibria

Phase region boundary  31 at:   6.645E-01  1.791E-01
    LIQUID
 ** GRAPHITE
Calculated                     42  equilibria

Phase region boundary  32 at:   6.125E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated                      6  equilibria

Phase region boundary  33 at:   6.125E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated.                     37  equilibria

Phase region boundary  34 at:   6.771E-01  2.438E-01
    LIQUID
 ** GRAPHITE
 ** M3C2

Phase region boundary  35 at:   3.771E-01  5.438E-01
    LIQUID
 ** M3C2
Calculated.                      2  equilibria

Phase region boundary  36 at:   3.711E-01  5.535E-01
    LIQUID
 ** M3C2
 ** M7C3

Phase region boundary  37 at:   3.211E-01  5.530E-01
    LIQUID
 ** M7C3
Calculated                     52  equilibria

Phase region boundary  38 at:   6.771E-01  2.438E-01
    LIQUID
 ** GRAPHITE
Calculated                     48  equilibria

Phase region boundary  39 at:   6.169E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated                      6  equilibria

Phase region boundary  40 at:   6.169E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated.                     40  equilibria

Phase region boundary  41 at:   6.845E-01  2.766E-01
    LIQUID
 ** GRAPHITE
 ** M3C2

Phase region boundary  42 at:   3.845E-01  5.766E-01
    LIQUID
 ** M3C2
Calculated.                      6  equilibria

Phase region boundary  43 at:   3.652E-01  6.202E-01
    LIQUID
 ** M3C2
 ** M7C3

Phase region boundary  44 at:   3.152E-01  6.637E-01
    LIQUID
 ** M7C3
Calculated                     37  equilibria

Phase region boundary  45 at:   6.845E-01  2.766E-01
    LIQUID
 ** GRAPHITE
Calculated                     55  equilibria

Phase region boundary  46 at:   6.214E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated                     22  equilibria

Phase region boundary  47 at:   6.214E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated                     66  equilibria

Phase region boundary  48 at:   6.259E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated                     22  equilibria

Phase region boundary  49 at:   6.259E-01  1.000E-02
    LIQUID
 ** GRAPHITE
Calculated                     62  equilibria

Phase region boundary  50 at:   5.307E-03  5.782E-01
    LIQUID
 ** BCC_A2
Calculated                     26  equilibria

Phase region boundary  51 at:   5.307E-03  5.782E-01
    LIQUID
 ** BCC_A2
Calculated                     54  equilibria

Phase region boundary  52 at:   5.190E-03  7.168E-01
    LIQUID
 ** BCC_A2
Calculated                     20  equilibria

Phase region boundary  53 at:   5.190E-03  7.168E-01
```

```
     LIQUID
  ** BCC_A2
 Calculated                      40  equilibria

 Phase region boundary  54 at:   5.138E-03  8.727E-01
     LIQUID
  ** BCC_A2
 Calculated                      26  equilibria

 Phase region boundary  55 at:   5.138E-03  8.727E-01
     LIQUID
  ** BCC_A2
 Calculated                      30  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\fecr
 c.POLY3
 CPU time for mapping                      4  seconds
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 3 T 1000 3000 8
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: se-con x(cr)=.6
   ... the command in full is SET_CONDITION
POLY_3: se-con x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-con t=1873
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7710 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: ad-ini 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liq
POLY_3:
POLY_3: map
 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16

 Phase region boundary   1 at:   5.118E-02  2.000E-02  1.446E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
 Terminating at diagram limit
 CALCULATED     7 EQUILIBRIA

 Phase region boundary   2 at:   5.118E-02  2.000E-02  1.446E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
 CALCULATED     6 EQUILIBRIA

 Phase region boundary   2 at:   8.299E-02  4.133E-02  1.467E+03
  ** LIQUID
  ** CEMENTITE
     FCC_A1
     M7C3

 Phase region boundary   2 at:   3.000E-01  2.339E-01  1.467E+03
  ** LIQUID
  ** CEMENTITE
     M7C3
 Terminating at known equilibrium
 CALCULATED     3 EQUILIBRIA

 Phase region boundary   2 at:   8.299E-02  4.133E-02  1.467E+03
  ** LIQUID
     FCC_A1
  ** M7C3
 CALCULATED    24 EQUILIBRIA

 Phase region boundary   2 at:   3.564E-02  2.106E-01  1.567E+03
  ** LIQUID
     BCC_A2
     FCC_A1
  ** M7C3

 Phase region boundary   2 at:   3.000E-01  5.271E-01  1.567E+03
  ** LIQUID
  ** BCC_A2
     M7C3
 *** SORRY CANNOT CONTINUE ***   17


 Phase region boundary   2 at:   3.564E-02  2.106E-01  1.567E+03
```

```
 ** LIQUID
 ** BCC_A2
    FCC_A1
Terminating at diagram limit
CALCULATED    35 EQUILIBRIA
SKIPPING LINE WITHOUT LIQUID#1
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   2.557E-02  2.000E-02  1.446E+03
 ** LIQUID
 ** CEMENTITE
    FCC_A1
Terminating at diagram limit
CALCULATED     7 EQUILIBRIA

Phase region boundary   2 at:   2.557E-02  2.000E-02  1.446E+03
 ** LIQUID
 ** CEMENTITE
    FCC_A1
Terminating at known equilibrium
CALCULATED     6 EQUILIBRIA

Phase region boundary   2 at:   2.160E-01  2.000E-02  1.456E+03
    LIQUID
 ** CEMENTITE
 ** GRAPHITE
Terminating at diagram limit
CALCULATED     9 EQUILIBRIA

Phase region boundary   2 at:   2.160E-01  2.000E-02  1.456E+03
    LIQUID
 ** CEMENTITE
 ** GRAPHITE
CALCULATED     8 EQUILIBRIA

Phase region boundary   2 at:   2.034E-01  5.587E-02  1.500E+03
    LIQUID
 ** CEMENTITE
 ** GRAPHITE
    M7C3
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   2.034E-01  5.587E-02  1.500E+03
    LIQUID
 ** CEMENTITE
 ** M7C3
Terminating at known equilibrium
CALCULATED     7 EQUILIBRIA

Phase region boundary   2 at:   2.034E-01  5.587E-02  1.500E+03
    LIQUID
 ** GRAPHITE
 ** M7C3
CALCULATED    55 EQUILIBRIA

Phase region boundary   2 at:   3.484E-01  4.662E-01  1.863E+03
    LIQUID
 ** GRAPHITE
    M3C2
 ** M7C3
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   3.484E-01  4.662E-01  1.863E+03
    LIQUID
 ** GRAPHITE
 ** M3C2
*** SORRY CANNOT CONTINUE ***    4

CALCULATED    33 EQUILIBRIA

Phase region boundary   2 at:   3.484E-01  4.662E-01  1.863E+03
    LIQUID
 ** M3C2
 ** M7C3
*** SORRY CANNOT CONTINUE ***    4

CALCULATED    28 EQUILIBRIA

Phase region boundary   2 at:   2.249E-01  2.000E-02  1.456E+03
    LIQUID
 ** CEMENTITE
 ** GRAPHITE
Terminating at diagram limit
CALCULATED     9 EQUILIBRIA

Phase region boundary   2 at:   2.249E-01  2.000E-02  1.456E+03
    LIQUID
 ** CEMENTITE
 ** GRAPHITE
Terminating at known equilibrium
CALCULATED     8 EQUILIBRIA

Phase region boundary   2 at:   2.338E-01  2.000E-02  1.456E+03
    LIQUID
 ** CEMENTITE
 ** GRAPHITE
Terminating at diagram limit
CALCULATED     9 EQUILIBRIA

Phase region boundary   2 at:   2.338E-01  2.000E-02  1.456E+03
    LIQUID
 ** CEMENTITE
 ** GRAPHITE
Terminating at known equilibrium
CALCULATED     8 EQUILIBRIA

Phase region boundary   2 at:   2.428E-01  2.000E-02  1.456E+03
    LIQUID
 ** CEMENTITE
 ** GRAPHITE
Terminating at diagram limit
CALCULATED     9 EQUILIBRIA

Phase region boundary   2 at:   2.428E-01  2.000E-02  1.456E+03
    LIQUID
 ** CEMENTITE
```

```
  ** GRAPHITE
 Terminating at known equilibrium
 CALCULATED     8 EQUILIBRIA

 Phase region boundary   2 at:   2.518E-01  2.000E-02  1.456E+03
     LIQUID
  ** CEMENTITE
  ** GRAPHITE
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA

 Phase region boundary   2 at:   2.518E-01  2.000E-02  1.456E+03
     LIQUID
  ** CEMENTITE
  ** GRAPHITE
 Terminating at known equilibrium
 CALCULATED     8 EQUILIBRIA

 Phase region boundary   2 at:   3.427E-02  6.000E-01  1.660E+03
     LIQUID
  ** BCC_A2
  ** M23C6
 CALCULATED    21 EQUILIBRIA

 Phase region boundary   2 at:   1.036E-01  4.168E-01  1.582E+03
     LIQUID
  ** BCC_A2
  ** M23C6
     M7C3
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   1.036E-01  4.168E-01  1.582E+03
     LIQUID
  ** BCC_A2
  ** M7C3
 Terminating at known equilibrium
 CALCULATED    13 EQUILIBRIA

 Phase region boundary   2 at:   1.036E-01  4.168E-01  1.582E+03
     LIQUID
  ** M23C6
  ** M7C3
 *** SORRY CANNOT CONTINUE ***    4

 CALCULATED    47 EQUILIBRIA

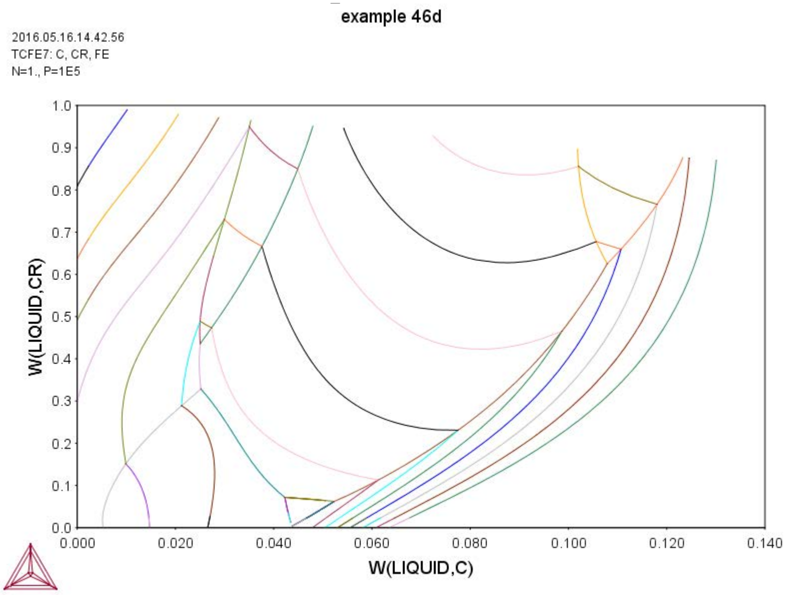
 Phase region boundary   2 at:   3.427E-02  6.000E-01  1.660E+03
     LIQUID
  ** BCC_A2
  ** M23C6
 *** SORRY CANNOT CONTINUE ***    4

 *** LAST BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\fecr
 c.POLY3
 CPU time for mapping                       2   seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x W(liquid,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(liquid,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Enter the table for the calculated data.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(liquid,c),W(liquid,cr),Temp_c;
POST:
POST: @@ Save the table on file
POST: tab tab1 fecrc_liq.tab
   ... the command in full is TABULATE
```

```
POST:
POST: @@ Set the axis variables and the axis text for the final diagram
POST: s-a-t-s x n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac C
POST: s-a-t-s y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac Cr
POST:
POST: s-d-a z temp-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-t-s z n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Temp C
POST:
POST: @@ Specify the diagram type to be traingular
POST: s-d-t y,,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST:
POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data
POST: @@ from the different tables created and saved. This is accomplished
POST: @@ using the command "CREATE_3D_DIAGRAM". Also define the scaling
POST: @@ to be used in the 3D-diagram.
POST: cre-3d
   ... the command in full is CREATE_3D_PLOTFILE
Use current WORKSPACE (WS), TAB files or BOTH: /WS/: BOTH
 The table must contain values for X,Y and Z axis
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    TEMP_C=T-273.15
 DEFINED TABLES
    TAB1=W(LIQUID,C), W(LIQUID,CR), TEMP_C
Table Name: tab1
Give TAB filename: /Cancel_to_finish/: fec_liq.tab fecr_liq.tab crc_liq.tab Cancel_to
Output file: /3Dplot/: tcex46_tri.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/: 1
Y-AXIS SCALING FROM 0.0 TO YMAX /1/: 1
Z-AXIS SCALING, GIVE ZMIN /0/: 1200
Z-AXIS SCALING, GIVE ZMAX /2000/: 4600

 It is possible to combine files by:
 Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

 Processing fec_liq.tab
  3.442910000000000E-009 <X<   1.00000000000000
  0.000000000000000E+000 <Y<  0.000000000000000E+000
   1153.44000000000      <Z<   4500.07000000000

 Processing fecr_liq.tab
  0.000000000000000E+000 <X<  0.000000000000000E+000
  1.174630000000000E-009 <Y<   1.00000000000000
   1515.56000000000      <Z<   1919.76000000000

 Processing crc_liq.tab
  3.441100000000000E-009 <X<   1.00000000000000
  3.343580000000000E-008 <Y<   1.00000000000000
   1533.06000000000      <Z<   4492.14000000000
POST: ,,,,,,,
  No such command, use HELP
POST:
POST: @@ Change the diagram type to obtain a squared diagram
POST: s-d-t n,,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST:
POST: @@ Create the squared 3D-diagram
POST: cre-3d
   ... the command in full is CREATE_3D_PLOTFILE
Use current WORKSPACE (WS), TAB files or BOTH: /WS/: BOTH
 The table must contain values for X,Y and Z axis
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    TEMP_C=T-273.15
 DEFINED TABLES
    TAB1=W(LIQUID,C), W(LIQUID,CR), TEMP_C
Table Name: tab1
Give TAB filename: /Cancel_to_finish/: fec_liq.tab fecr_liq.tab crc_liq.tab Cancel_to
Output file: /3Dplot/: tcex46_sqrt.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/: .12
Y-AXIS SCALING FROM 0.0 TO YMAX /1/: 1
Z-AXIS SCALING, GIVE ZMIN /0/: 1200
Z-AXIS SCALING, GIVE ZMAX /2000/: 2200

 It is possible to combine files by:
 Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

 Processing fec_liq.tab
  3.442910000000000E-009 <X<   1.00000000000000
  0.000000000000000E+000 <Y<  0.000000000000000E+000
   1153.44000000000      <Z<   4500.07000000000

 Processing fecr_liq.tab
  0.000000000000000E+000 <X<  0.000000000000000E+000
  1.174630000000000E-009 <Y<   1.00000000000000
   1515.56000000000      <Z<   1919.76000000000

 Processing crc_liq.tab
  3.441100000000000E-009 <X<   1.00000000000000
  3.343580000000000E-008 <Y<   1.00000000000000
   1533.06000000000      <Z<   4492.14000000000
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex47

```
About Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex47.TCM"SYS: set-echo
SYS: @@
SYS: @@ 3D-Diagram
SYS: @@ A quarternay diagram with the gamma volume in the
SYS: @@ Fe-Cr-Ni-C system at 1373K
SYS: @@
SYS: @@ This file calculated the gamma volume in fe-cr-ni-c systeam at 1100C
SYS: @@ Please note that in order to view the generated file, tcex47.wrl,
SYS: @@ it's necessary to install a WRML(Wirtual Reality Modelling
SYS: @@ Language) viewer to web browser in use. WRML viwers can be
SYS: @@ downloaded witout any cost from e.g. www.parallelgraphics.com
SYS: @@ and www.sim.no
SYS:
SYS: set-log ex47
Heading:
SYS: @@ Calculate the Fe-Cr-C side of the diagram
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw FEDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database

 VA                      /-  DEFINED
TDB_FEDEMO: rej-sys
   ... the command in full is REJECT
 VA                      /-  DEFINED
 REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
   DEFINED
TDB_FEDEMO: rej-ph * all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                BCC_A2
 CEMENTITE               CHI_A12                 DIAMOND_FCC_A4
 FCC_A1                  GRAPHITE                HCP_A3
 KSI_CARBIDE             LAVES_PHASE_C14         M23C6
 M3C2                    M5C2                    M7C3
 SIGMA  REJECTED
TDB_FEDEMO: res-ph fcc_a1,bcc_a2,m23,m7,cementite
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  M23C6
 M7C3                    CEMENTITE  RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.05
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          5731 grid points in               0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
```

```
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 1,,,,,
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   1.765E-01  1.880E-01
     FCC_A1
  ** M7C3
 Calculated.                      5  equilibria

 Phase region boundary   2 at:   1.830E-01  1.507E-01
  ** CEMENTITE
     FCC_A1
  ** M7C3

 Phase region boundary   3 at:   1.580E-01  9.227E-02
  ** CEMENTITE
     FCC_A1
 Calculated                     25  equilibria

 Phase region boundary   4 at:   1.830E-01  1.507E-01
     FCC_A1
  ** M7C3
 Calculated.                     23  equilibria

 Phase region boundary   5 at:   1.589E-01  3.687E-01
     FCC_A1
  ** M23C6
  ** M7C3

 Phase region boundary   6 at:   1.123E-01  3.478E-01
     FCC_A1
  ** M23C6
 Calculated.                      2  equilibria

 Phase region boundary   7 at:   1.122E-01  3.494E-01
  ** BCC_A2
     FCC_A1
  ** M23C6

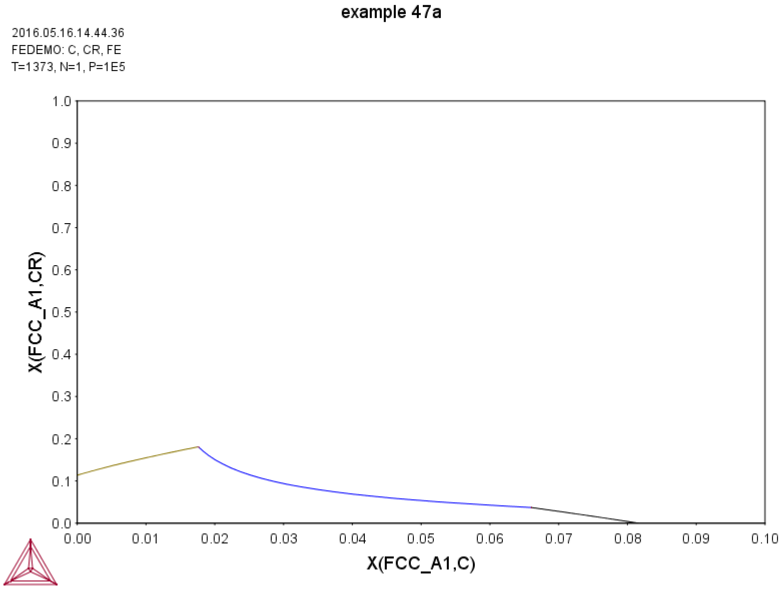
 Phase region boundary   8 at:   1.066E-02  1.975E-01
  ** BCC_A2
     FCC_A1
 Calculated                     23  equilibria

 Phase region boundary   9 at:   1.765E-01  1.880E-01
     FCC_A1
  ** M7C3
 Calculated.                     20  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
 47.POLY3
 CPU time for mapping                     0  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x x(fcc_a1,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 47a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second Ni content which is "zero"
POST: @@ here, and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),ZERO,x(fcc_a1,c)
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fecrc_1373.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Fe-Cr-ni side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
   ... the command in full is REJECT
 VA                       /-  DEFINED
 REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr ni
   ... the command in full is DEFINE_SYSTEM
 FE                       CR                       NI
   DEFINED
TDB_FEDEMO: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L                 BCC_A2                   CHI_A12
 FCC_A1                   HCP_A3                   LAVES_PHASE_C14
 SIGMA  REJECTED
TDB_FEDEMO: res-ph bcc_a2,fcc_a1
   ... the command in full is RESTORE
 BCC_A2                   FCC_A1  RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.005
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           3954 grid points in               0 s
Found the set of lowest grid points in                 0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(ni) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
```

```
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Working hard
 Generating start point   1
 Generating start point   2

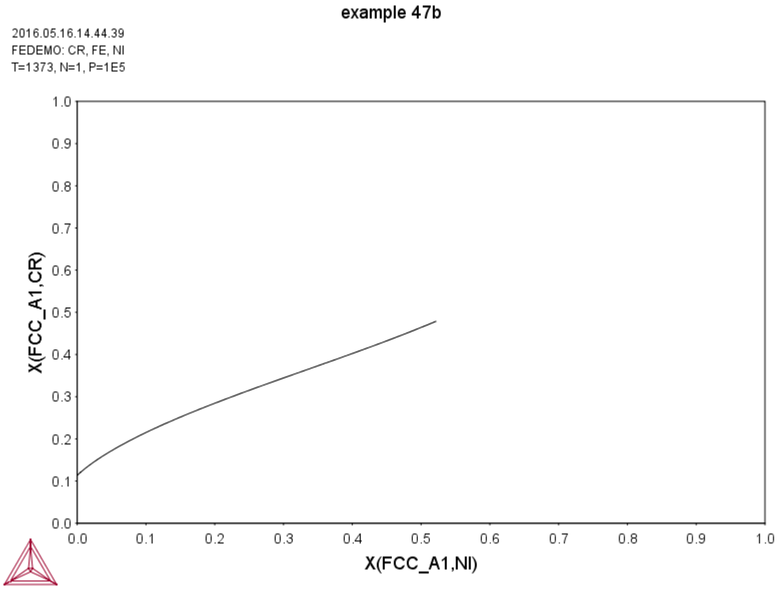
 Phase region boundary   1 at:   4.206E-03  1.318E-01
  ** BCC_A2
     FCC_A1
 Calculated                     12  equilibria

 Phase region boundary   2 at:   4.206E-03  1.318E-01
  ** BCC_A2
     FCC_A1
 Calculated                     86  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
 47.POLY3
 CPU time for mapping                     1  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x x(fcc_a1,ni)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 47b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second Ni content
POST: @@ and in the last column the C content of the fcc_a1 phase, which is zero
POST: e-sym tab tab2
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),x(fcc_a1,ni),zero
&
POST: @@ Save the tabulated data on file
POST: tab tab2 fecrni_1373.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Fe-C-Ni side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
   ... the command in full is REJECT
 VA                        /-  DEFINED
 REINITIATING GES5 .....
```

```
TDB_FEDEMO: de-sys fe Ni C
   ... the command in full is DEFINE_SYSTEM
 FE                      NI                       C
   DEFINED
TDB_FEDEMO: rej-ph * all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                 BCC_A2
 CEMENTITE               DIAMOND_FCC_A4           FCC_A1
 GRAPHITE                HCP_A3                   KSI_CARBIDE
 LAVES_PHASE_C14         M23C6                    M5C2
 M7C3  REJECTED
TDB_FEDEMO: res-ph fcc_a1,bcc_a2,cementite,hcp_a3
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                   CEMENTITE
 HCP_A3  RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (parameters listed in Calphad, 11 (1987), 203-218); C-NI'
  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'A. Gabriel, P. Gustafson, and I. Ansara, Calphad, 11 (1987), 203 -218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'A. Fernandez Guillermet, Z. Metallkde., 79 (1988), 524-536, TRITA -MAC
      362 (1988); C-CO-NI AND C-CO-FE-NI'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          5594 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(ni) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3:
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

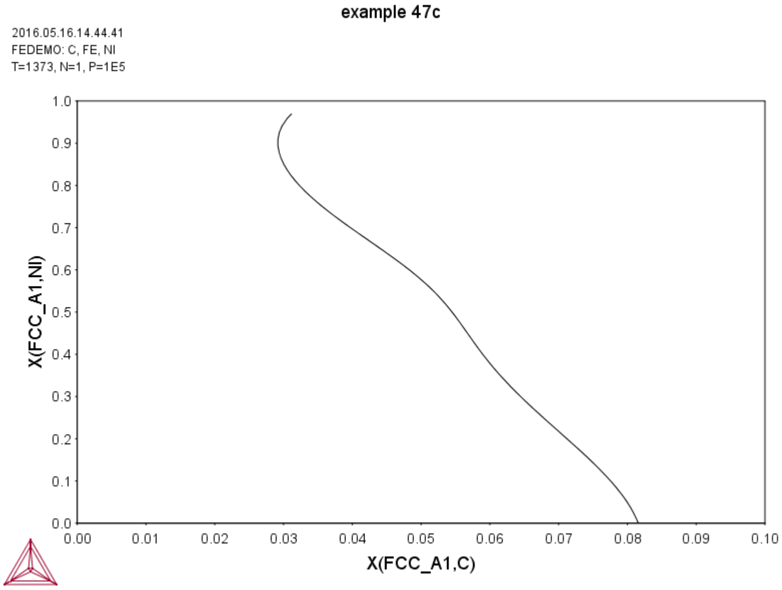
 Phase region boundary   1 at:   1.657E-01  3.147E-03
  ** CEMENTITE
     FCC_A1
 Calculated                      9  equilibria

 Phase region boundary   2 at:   1.657E-01  3.147E-03
  ** CEMENTITE
     FCC_A1
 Calculated                    104  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
 47.POLY3
 CPU time for mapping                      0  seconds
POLY_3:
POLY_3: post
```

```
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x x(fcc_a1,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,ni)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 47c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second Ni
POST: @@ and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab3
   ... the command in full is ENTER_SYMBOL
Variable(s): zero,x(fcc_a1,ni),x(fcc_a1,c)
&
POST: @@ Save the tabulated data on file
POST: tab tab3 fenic_1373.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Cr-ni-C side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
   ... the command in full is REJECT
 VA                       /-  DEFINED
 REINITIATING GES5 .....
TDB_FEDEMO: de-sys cr ni C
   ... the command in full is DEFINE_SYSTEM
 CR                       NI                       C
   DEFINED
TDB_FEDEMO:
TDB_FEDEMO: rej-ph * all
   ... the command in full is REJECT
 GAS:G                    LIQUID:L                 BCC_A2
 CEMENTITE                CHI_A12                  DIAMOND_FCC_A4
 FCC_A1                   GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          M23C6
 M3C2                     M7C3                     SIGMA
   REJECTED
TDB_FEDEMO: res-ph fcc_a1,bcc_a2,cementite,hcp_a3
   ... the command in full is RESTORE
 FCC_A1                   BCC_A2                   CEMENTITE
 HCP_A3  RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (parameters listed in Calphad, 11 (1987), 203-218); C-NI'
  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'NPL, unpublished work (1989); C-Cr-Ni'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
```

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      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'A. Gabriel, P. Gustafson, and I. Ansara, Calphad, 11 (1987), 203 -218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
  'A. Fernandez Guillermet, Z. Metallkde., 79 (1988), 524-536, TRITA -MAC
      362 (1988); C-CO-NI AND C-CO-FE-NI'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.005
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          5594 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3:
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   1.410E-01  4.254E-03
  ** CEMENTITE
     FCC_A1
 Calculated                     10  equilibria

 Phase region boundary   2 at:   1.410E-01  4.254E-03
  ** CEMENTITE
     FCC_A1
 Calculated.                     14  equilibria

 Phase region boundary   3 at:   1.475E-01  1.250E-01
  ** CEMENTITE
     FCC_A1
  ** FCC_A1#2

 Phase region boundary   4 at:   2.681E-01  3.002E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                      7  equilibria
 Calculated                      7  equilibria

 Phase region boundary   5 at:   2.681E-01  3.002E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                      4  equilibria

 Phase region boundary   6 at:   2.545E-01  3.227E-01
     FCC_A1
  ** FCC_A1#2
  ** HCP_A3

 Phase region boundary   7 at:   1.819E-01  3.945E-01
     FCC_A1
  ** HCP_A3
 Calculated.                     14  equilibria

 Phase region boundary   8 at:   1.520E-01  5.236E-01
  ** CEMENTITE
     FCC_A1
  ** HCP_A3

 Phase region boundary   9 at:   1.267E-01  5.426E-01
  ** CEMENTITE
     FCC_A1
 Calculated.                      8  equilibria

 Phase region boundary  10 at:   1.262E-01  6.075E-01
  ** BCC_A2
  ** CEMENTITE
     FCC_A1

 Phase region boundary  11 at:   1.249E-03  6.835E-01
```

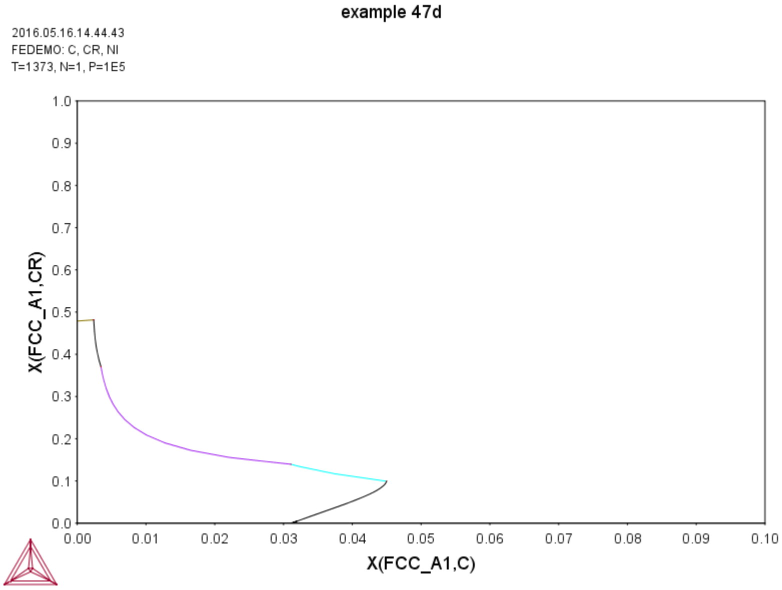
```
  ** BCC_A2
     FCC_A1
 Calculated                     13  equilibria

 Phase region boundary  12 at:   1.475E-01  1.250E-01
  ** CEMENTITE
     FCC_A1
 Calculated                     27  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
 47.POLY3
 CPU time for mapping                     0  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x x(fcc_a1,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 47d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second Ni content
POST: @@ and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab4
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),x(fcc_a1,ni),x(fcc_a1,c)
&
POST: @@ Save the tabulated data on file
POST: tab tab4 crnic_1373.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3:
POLY_3: @@ Next calculate a projection of the Fe-Cr-ni-C system
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
   ... the command in full is REJECT
 VA                       /-  DEFINED
 REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr ni C
   ... the command in full is DEFINE_SYSTEM
 FE                       CR                       NI
 C  DEFINED
TDB_FEDEMO: rej-ph * all
   ... the command in full is REJECT
 GAS:G                    LIQUID:L                 BCC_A2
 CEMENTITE                CHI_A12                  DIAMOND_FCC_A4
 FCC_A1                   GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          M23C6
 M3C2                     M5C2                     M7C3
 SIGMA  REJECTED
TDB_FEDEMO: res-ph fcc_a1,bcc_a2,hcp_a3,m23,fcc_a1,bcc_a2,m23,m7,cementite
   ... the command in full is RESTORE
 FCC_A1                   BCC_A2                   HCP_A3
 M23C6                    M7C3                     CEMENTITE
   RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
```

```
 FUNCTIONS ....

 List of references for assessed data

  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (parameters listed in Calphad, 11 (1987), 203-218); C-NI'
  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
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  'A. Gabriel, P. Gustafson, and I. Ansara, Calphad, 11 (1987), 203 -218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
  'A. Fernandez Guillermet, Z. Metallkde., 79 (1988), 524-536, TRITA -MAC
      362 (1988); C-CO-NI AND C-CO-FE-NI'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, Vol.
      53, pp. 105-125; Molar volumes'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.02
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          9750 grid points in              0 s
    33 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .005
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(ni) 0 1 .005
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.04
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    15 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.06
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    22 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.08
   ... the command in full is SET_CONDITION
```
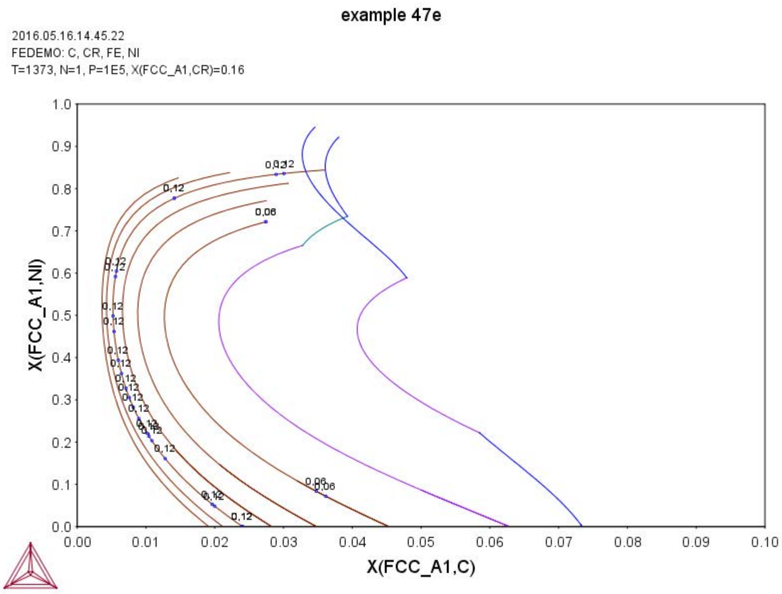

```
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    17 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    17 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.12
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    17 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.14
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    18 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.16c-e
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 ERROR                  1611  when calculating equilibrium
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 ERROR                  1611  when calculating equilibrium
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
```

```
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard

Phase region boundary   1 at:   5.000E-02  2.951E-01
    FCC_A1
 ** M7C3
Calculated.                      60  equilibria

Phase region boundary   2 at:   4.791E-02  5.888E-01
 ** CEMENTITE
    FCC_A1
 ** M7C3

Phase region boundary   3 at:   4.791E-02  5.888E-01
    CEMENTITE
    FCC_A1
 ** M7C3
Calculated.                      38  equilibria
Terminating at known equilibrium

Phase region boundary   4 at:   4.791E-02  5.888E-01
 ** CEMENTITE
    FCC_A1
Calculated                      86  equilibria

Phase region boundary   5 at:   4.791E-02  5.888E-01
 ** CEMENTITE
    FCC_A1
    M7C3
Calculated.                      87  equilibria
Terminating at known equilibrium

Phase region boundary   6 at:   4.791E-02  5.888E-01
    FCC_A1
 ** M7C3
Calculated.                      75  equilibria

Phase region boundary   7 at:   5.851E-02  2.219E-01
 ** CEMENTITE
    FCC_A1
 ** M7C3

Phase region boundary   8 at:   5.851E-02  2.219E-01
    CEMENTITE
    FCC_A1
 ** M7C3
Calculated.                      69  equilibria
Terminating at known equilibrium

Phase region boundary   9 at:   5.851E-02  2.219E-01
 ** CEMENTITE
    FCC_A1
Calculated                      60  equilibria

Phase region boundary  10 at:   5.851E-02  2.219E-01
 ** CEMENTITE
    FCC_A1
    M7C3
Calculated.                      79  equilibria
Terminating at known equilibrium

Phase region boundary  11 at:   5.000E-02  2.951E-01
    FCC_A1
 ** M7C3
Calculated.                      16  equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   7.320E-02  5.000E-03
 ** CEMENTITE
    FCC_A1
Calculated                      22  equilibria

Phase region boundary  13 at:   7.320E-02  5.000E-03
 ** CEMENTITE
    FCC_A1
Calculated.                      45  equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   5.000E-02  8.665E-02
    FCC_A1
 ** M7C3
Calculated.                     117  equilibria

Phase region boundary  15 at:   3.277E-02  6.655E-01
    FCC_A1
 ** FCC_A1#2
 ** M7C3

Phase region boundary  16 at:   3.277E-02  6.655E-01
    FCC_A1
    FCC_A1#2
 ** M7C3
Calculated.                     134  equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   3.277E-02  6.655E-01
    FCC_A1
 ** FCC_A1#2
Calculated.                      15  equilibria

Phase region boundary  18 at:   3.930E-02  7.344E-01
 ** CEMENTITE
    FCC_A1
 ** FCC_A1#2

Phase region boundary  19 at:   3.930E-02  7.344E-01
    CEMENTITE
    FCC_A1
 ** FCC_A1#2
Calculated.                      64  equilibria
Terminating at known equilibrium
```

```
Phase region boundary  20 at:   3.930E-02  7.344E-01
 ** CEMENTITE
    FCC_A1
Calculated                     49  equilibria

Phase region boundary  21 at:   3.930E-02  7.344E-01
 ** CEMENTITE
    FCC_A1
    FCC_A1#2
Calculated.                    147  equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   3.277E-02  6.655E-01
    FCC_A1
 ** FCC_A1#2
    M7C3
Calculated.                    108  equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   3.277E-02  6.655E-01
    FCC_A1
 ** M7C3
Calculated                    145  equilibria

Phase region boundary  24 at:   5.000E-02  8.665E-02
    FCC_A1
 ** M7C3
Calculated                     32  equilibria

Phase region boundary  25 at:   6.207E-02  5.000E-03
    FCC_A1
 ** M7C3
Calculated                      5  equilibria

Phase region boundary  26 at:   6.207E-02  5.000E-03
    FCC_A1
 ** M7C3
Calculated.                    134  equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.000E-01  5.000E-03
 ** FCC_A1
    M7C3
Calculated                     10  equilibria

Phase region boundary  28 at:   3.000E-01  5.000E-03
 ** FCC_A1
    M7C3
Calculated.                     44  equilibria

Phase region boundary  29 at:   3.000E-01  1.229E-01
 ** FCC_A1
 ** FCC_A1#2
    M7C3

Phase region boundary  30 at:   3.000E-01  1.229E-01
 ** FCC_A1
    FCC_A1#2
    M7C3
Calculated.                     48  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   3.000E-01  1.229E-01
    FCC_A1
 ** FCC_A1#2
    M7C3
Calculated.                    121  equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   3.000E-01  1.229E-01
 ** FCC_A1
    M7C3
Calculated                     65  equilibria

Phase region boundary  33 at:   3.000E-01  5.000E-03
 ** FCC_A1
    M7C3
Calculated                     11  equilibria

Phase region boundary  34 at:   3.000E-01  5.000E-03
 ** FCC_A1
    M7C3
Calculated.                     45  equilibria

Phase region boundary  35 at:   3.000E-01  1.251E-01
 ** FCC_A1
 ** FCC_A1#2
    M7C3

Phase region boundary  36 at:   3.000E-01  1.251E-01
 ** FCC_A1
    FCC_A1#2
    M7C3
Calculated.                     49  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   3.000E-01  1.251E-01
    FCC_A1
 ** FCC_A1#2
    M7C3
Calculated.                    131  equilibria
Terminating at known equilibrium

Phase region boundary  38 at:   3.000E-01  1.251E-01
 ** FCC_A1
    M7C3
Calculated                     63  equilibria

Phase region boundary  39 at:   3.000E-01  5.000E-03
 ** FCC_A1
    M7C3
Calculated                     11  equilibria

Phase region boundary  40 at:   3.000E-01  5.000E-03
 ** FCC_A1
```

```
     M7C3
 Calculated.                      46  equilibria

 Phase region boundary  41 at:   3.000E-01  1.310E-01
  ** FCC_A1
  ** FCC_A1#2
     M7C3

 Phase region boundary  42 at:   3.000E-01  1.310E-01
  ** FCC_A1
     FCC_A1#2
     M7C3
 Calculated.                      51  equilibria
 Terminating at known equilibrium

 Phase region boundary  43 at:   3.000E-01  1.310E-01
     FCC_A1
  ** FCC_A1#2
     M7C3
 Calculated.                     138  equilibria
 Terminating at known equilibrium

 Phase region boundary  44 at:   3.000E-01  1.310E-01
  ** FCC_A1
     M7C3
 Calculated                      62  equilibria

 Phase region boundary  45 at:   3.000E-01  5.000E-03
  ** FCC_A1
     M7C3
 Calculated                      33  equilibria

 Phase region boundary  46 at:   3.000E-01  5.000E-03
  ** FCC_A1
     M7C3
 Calculated                      63  equilibria

 Phase region boundary  47 at:   3.000E-01  5.000E-03
  ** FCC_A1
     M7C3
 Calculated                      19  equilibria

 Phase region boundary  48 at:   3.000E-01  5.000E-03
  ** FCC_A1
     M7C3
 Calculated                      50  equilibria

 Phase region boundary  49 at:   3.000E-01  5.000E-03
  ** FCC_A1
     M7C3
 Calculated                      19  equilibria

 Phase region boundary  50 at:   3.000E-01  5.000E-03
  ** FCC_A1
     M7C3
 Calculated                      51  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
 47.POLY3
 CPU time for mapping                     10  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x x(fcc_a1,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,ni)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z x(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-a-t-s y y
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s x y
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s z y
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-s-s x n 0 0.1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s z n 0 1
   ... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 47e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second ni content
POST: @@ and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab5
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),x(fcc_a1,ni),x(fcc_a1,c)
&
POST: @@ Save the tabulated data on file
POST: tab tab5 fecrnic_1373.tab
   ... the command in full is TABULATE
POST:
POST:
POST: back
POLY_3: rei,,,,
   ... the command in full is REINITIATE_MODULE
POLY_3:
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.001
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.01
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          9750 grid points in              0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .001
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(ni) 0 1 .001
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 1,,,
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(cr)=.05
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add-in 1,,,
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(cr)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1,,,
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
```

```
 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6

 Phase region boundary   1 at:   7.757E-02  1.000E-03
  ** CEMENTITE
     FCC_A1
 Calculated                      8  equilibria

 Phase region boundary   2 at:   7.757E-02  1.000E-03
  ** CEMENTITE
     FCC_A1
 Calculated                    969  equilibria

 Phase region boundary   3 at:   5.282E-02  1.000E-03
     FCC_A1
  ** M7C3
 Calculated                     15  equilibria

 Phase region boundary   4 at:   5.282E-02  1.000E-03
     FCC_A1
  ** M7C3
 Calculated.                    694  equilibria

 Phase region boundary   5 at:   2.910E-02  6.938E-01
     FCC_A1
  ** FCC_A1#2
  ** M7C3

 Phase region boundary   6 at:   2.910E-02  6.938E-01
     FCC_A1
     FCC_A1#2
  ** M7C3
 Calculated.                     95  equilibria

 Phase region boundary   7 at:   7.037E-02  6.004E-01
  ** CEMENTITE
     FCC_A1
     FCC_A1#2
  ** M7C3

 Phase region boundary   8 at:   1.432E-01  5.581E-01
     CEMENTITE
     FCC_A1
  ** FCC_A1#2
 Calculated.                    214  equilibria

 Phase region boundary   9 at:   3.838E-02  7.703E-01
  ** CEMENTITE
     FCC_A1
  ** FCC_A1#2

 Phase region boundary  10 at:   3.838E-02  7.703E-01
     FCC_A1
  ** FCC_A1#2
 Calculated.                     78  equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   3.838E-02  7.703E-01
  ** CEMENTITE
     FCC_A1
 Calculated                    156  equilibria

 Phase region boundary  12 at:   3.838E-02  7.703E-01
  ** CEMENTITE
     FCC_A1
     FCC_A1#2
 Calculated.                    171  equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   1.432E-01  5.581E-01
     CEMENTITE
     FCC_A1
  ** M7C3
 Calculated                    582  equilibria

 Phase region boundary  14 at:   7.104E-02  5.895E-01
  ** CEMENTITE
     FCC_A1
     M7C3
 Calculated                    603  equilibria

 Phase region boundary  15 at:   7.104E-02  5.895E-01
     FCC_A1
  ** FCC_A1#2
     M7C3
 Calculated.                    106  equilibria
 Terminating at known equilibrium

 Phase region boundary  16 at:   2.910E-02  6.938E-01
     FCC_A1
  ** M7C3
 Calculated                    707  equilibria

 Phase region boundary  17 at:   2.819E-02  1.000E-03
     FCC_A1
  ** M7C3
 Calculated                      8  equilibria

 Phase region boundary  18 at:   2.819E-02  1.000E-03
     FCC_A1
  ** M7C3
 Calculated.                    813  equilibria

 Phase region boundary  19 at:   3.066E-02  8.126E-01
     FCC_A1
  ** FCC_A1#2
  ** M7C3
```

```
 Phase region boundary  20 at:   3.066E-02  8.126E-01
     FCC_A1
     FCC_A1#2
  ** M7C3
 Calculated.                    290  equilibria
 Terminating at known equilibrium

 Phase region boundary  21 at:   3.066E-02  8.126E-01
     FCC_A1
  ** FCC_A1#2
 Calculated                      58  equilibria

 Phase region boundary  22 at:   3.066E-02  8.126E-01
     FCC_A1
  ** FCC_A1#2
     M7C3
 Calculated.                    324  equilibria
 Terminating at known equilibrium

 Phase region boundary  23 at:   3.066E-02  8.126E-01
     FCC_A1
  ** M7C3
 Calculated                     822  equilibria
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
 47.POLY3
 CPU time for mapping                     12  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST:
POST: se-d-t n y,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second ni
POST: @@ and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab6
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),x(fcc_a1,ni),x(fcc_a1,c)
&
POST: se-tit
   ... the command in full is SET_TITLE
TITLE : Fe-Cr-Ni-C system
POST: s-d-a x x(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,ni)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z x(fcc_a1,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-a-t-s x n X(Cr)
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s y n X(Ni)
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s z n X(C)
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data
POST: @@ from the different tables created and saved. This is accomplished
POST: @@ using the command "CREATE_3D_DIAGRAM". Also define the scaling
POST: @@ to be used in the 3D-diagram.
POST: cre BOTH tab6
   ... the command in full is CREATE_3D_PLOTFILE
 The table must contain values for X,Y and Z axis
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    TEMP_C=T-273.15
 DEFINED TABLES
    TAB6=X(FCC_A1,CR), X(FCC_A1,NI), X(FCC_A1,C)
Give TAB filename: /Cancel_to_finish/: fecrc_1373.tab fecrni_1373.tab fenic_1373.tab crnic_1373.tab fecrnic_1373.tab Cancel_to
Output file: /3Dplot/: tcex47.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/: 1
Y-AXIS SCALING FROM 0.0 TO YMAX /1/: 1
 TETRAHEDRON DIAGRAM, ZMIN SET 0.0
Z-AXIS SCALING, GIVE ZMAX /2000/: .5

 It is possible to combine files by:
 Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

 Processing fecrc_1373.tab
  5.287230000000000E-009 <X<  0.180692000000000
  0.000000000000000E+000 <Y<  0.000000000000000E+000
  6.987710000000000E-009 <Z<  8.158250000000000E-002

 Processing fecrni_1373.tab
  0.113628000000000      <X<  0.478622000000000
  2.068240000000000E-008 <Y<  0.521377000000000
  0.000000000000000E+000 <Z<  0.000000000000000E+000

 Processing fenic_1373.tab
  0.000000000000000E+000 <X<  0.000000000000000E+000
  1.100300000000000E-008 <Y<  0.968861000000000
  2.918660000000000E-002 <Z<  8.158250000000000E-002

 Processing crnic_1373.tab
  7.671840000000000E-010 <X<  0.481628000000000
  0.515966000000000      <Y<  0.968861000000000
  1.000000000000000E-012 <Z<  4.498370000000000E-002

 Processing fecrnic_1373.tab
  2.000000000000000E-002 <X<  0.160000000000000
  9.371880000000000E-013 <Y<  0.945434000000000
  3.608350000000000E-003 <Z<  7.342520000000000E-002
POST:
POST: se-inter
   ... the command in full is SET_INTERACTIVE_MODE
```

POST:

tcex48

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex48\tcex48.TCM"SYS: set-echo
SYS: @@
SYS: @@ Scheil solidification with C back diffusion in solid phases and comparison with simple Scheil and equilibrium calculations.
SYS: @@
SYS: @@  Scheil solidification with C back diffusion (ScheiC) in solid phases
SYS: @@                                   and
SYS: @@ comparison with simple Scheil and equilibrium calculations
SYS: @@
SYS: set-log ex48,,,
SYS: @@ use system command delete old exp files if any
SYS: @@ for unix
SYS: @@ rm *.exp
SYS: @@ for pc
SYS: @del *.exp
Det g?r inte att hitta c:\jenkins\WORKSP~1\THERMO~1\examples\tcex48\*.exp.
SYS: @@
SYS: @@ first do ScheiC by assigning C as fast diffuse element
SYS: @@ plot solidification and microsegregation diagram and save them
SYS: @@ to files
SYS: @@
SYS: go scheil
   ... the command in full is GOTO_MODULE
SCHEIL: save-file-name tcex48a
SCHEIL: start
   ... the command in full is START_WIZARD
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
Database /TCFE8/: FEDEMO
 Current database: Iron Demo Database

 VA                       /-  DEFINED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 1
2nd alloying element: cr 10
Next alloying element:
Temperature (C) /2000/: 2000
 VA                       /-  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED


 This database has following phases for the defined system

 GAS:G                     LIQUID:L                  BCC_A2
 CEMENTITE                 CHI_A12                   DIAMOND_FCC_A4
 FCC_A1                    GRAPHITE                  HCP_A3
 KSI_CARBIDE               LAVES_PHASE_C14           M23C6
 M3C2                      M5C2                      M7C3
 SIGMA

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

 ........................................................

    The following phases are retained in this system:

 GAS:G                     LIQUID:L                  BCC_A2
 CEMENTITE                 CHI_A12                   DIAMOND_FCC_A4
 FCC_A1                    GRAPHITE                  HCP_A3
 KSI_CARBIDE               LAVES_PHASE_C14           M23C6
 M3C2                      M5C2                      M7C3
 SIGMA

 ........................................................

OK? /Y/: Y
 GAS:G  REJECTED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
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  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
```
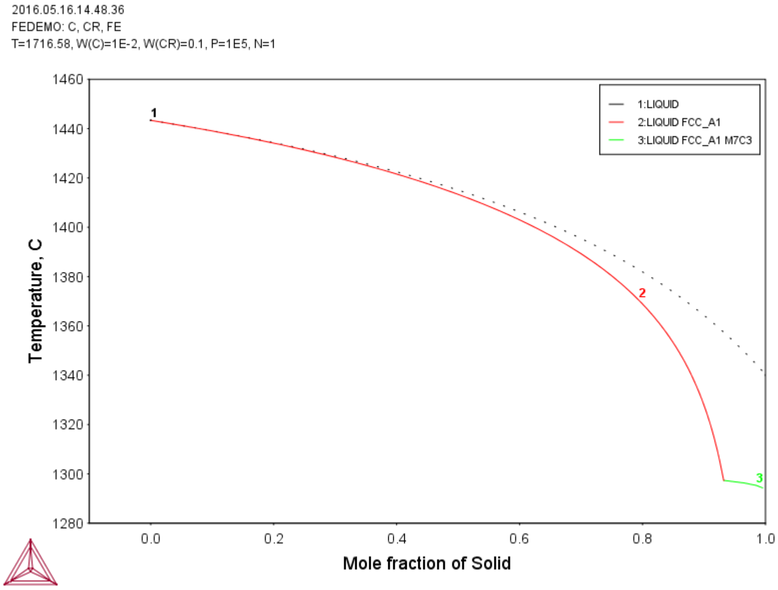
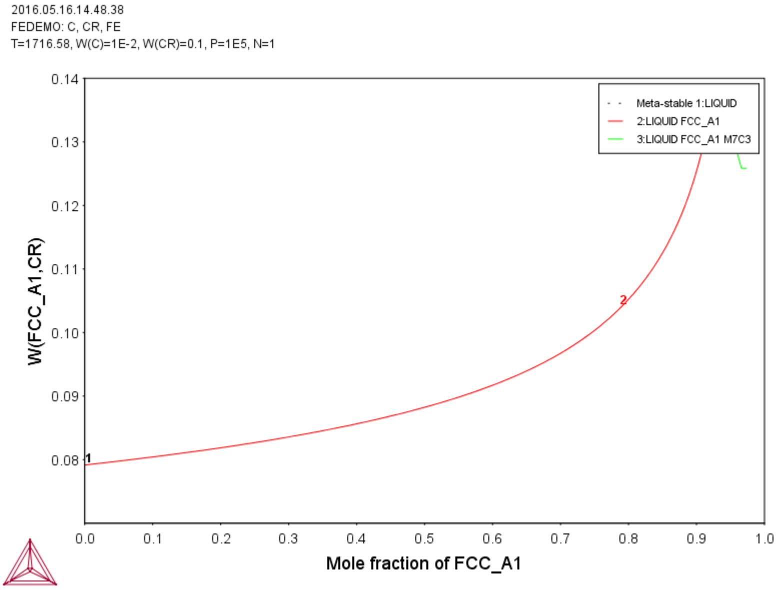

```
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
      (1986); CR-FE-MO'
  'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, estimated parameter 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
Should any phase have a miscibility gap check? /N/: N
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/: C
   ... the command in full is SET_NUMERICAL_LIMITS
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=2273.15, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1    DEGREES OF FREEDOM 0
To form FCC_A1#1 the condition is set to T=1716.48507839
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
   ... the command in full is ADVANCED_OPTIONS
   ... the command in full is STEP_WITH_OPTIONS
...OK

 Phase Region from    1716.48     for:
     LIQUID
     FCC_A1
 Global check of removing phase at  1.71649E+03
 Calculated     3 equilibria

 Phase Region from    1716.49     for:
     LIQUID
 Terminating at    1716.58
 Calculated     4 equilibria

 Phase Region from    1716.48     for:
     LIQUID
     FCC_A1
 Global test at  1.70848E+03 .... OK
 Global test at  1.69848E+03 .... OK
 Global test at  1.68848E+03 .... OK
 Global test at  1.67848E+03 .... OK
 Global test at  1.66848E+03 .... OK
 Global test at  1.65848E+03 .... OK
 Global test at  1.64848E+03 .... OK
 Global test at  1.63848E+03 .... OK
 Global test at  1.62848E+03 .... OK
 Global test at  1.61848E+03 .... OK
 Global check of removing phase at  1.61342E+03
 Calculated   106 equilibria

 Phase Region from    1613.42     for:
     FCC_A1
 Calculated     4 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex48\tcex
 48a.POLY3

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes


  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

   ... the command in full is ENTER_SYMBOL
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 An EXP file c:\jenkins\WORKSP~1\THERMO~1\examples\tcex48\tcex48a_EQ.EXP
 has been created to store the equilibrium solidification results.
   ... the command in full is READ_WORKSPACES
  CALCULATING SCHEIL SOLIDFICATION
   ... the command in full is SET_NUMERICAL_LIMITS

     T(C)      fraction solid

   1443.425       0.000000

  PHASE REGION:LIQUID + FCC_A1

     T(C)      fraction solid

   1443.331       0.000000
   1442.331      0.2475817E-01
   1441.331      0.4847108E-01
   1440.331      0.7146723E-01
   1439.331      0.9377411E-01
   1438.331      0.1154198
   1437.331      0.1364307
   1436.331      0.1568321
   1435.331      0.1766476
   1434.331      0.1958998
   1433.331      0.2146101
   1432.331      0.2327987
   1431.331      0.2504848
   1430.331      0.2676869
   1429.331      0.2844222
   1428.331      0.3007072
   1427.331      0.3165578
   1426.331      0.3319888
   1425.331      0.3470146
   1424.331      0.3616488
   1423.331      0.3759043
   1422.331      0.3897936
   1421.331      0.4033284
```

1420.331	0.4165201
1419.331	0.4293794
1418.331	0.4419167
1417.331	0.4541419
1416.331	0.4660643
1415.331	0.4776932
1414.331	0.4890371
1413.331	0.5001044
1412.331	0.5109030
1411.331	0.5214407
1410.331	0.5317247
1409.331	0.5417621
1408.331	0.5515598
1407.331	0.5611242
1406.331	0.5704616
1405.331	0.5795781
1404.331	0.5884795
1403.331	0.5971714
1402.331	0.6056592
1401.331	0.6139481
1400.331	0.6220433
1399.331	0.6299494
1398.331	0.6376713
1397.331	0.6452135
1396.331	0.6525803
1395.331	0.6597760
1394.331	0.6668048
1393.331	0.6736706
1392.331	0.6803774
1391.331	0.6869287
1390.331	0.6933284
1389.331	0.6995799
1388.331	0.7056866
1387.331	0.7116520
1386.331	0.7174792
1385.331	0.7231714
1384.331	0.7287317
1383.331	0.7341631
1382.331	0.7394684
1381.331	0.7446507
1380.331	0.7497126
1379.331	0.7546568
1378.331	0.7594860
1377.331	0.7642028
1376.331	0.7688097
1375.331	0.7733092
1374.331	0.7777037
1373.331	0.7819955
1372.331	0.7861870
1371.331	0.7902805
1370.331	0.7942781
1369.331	0.7981819
1368.331	0.8019943
1367.331	0.8057171
1366.331	0.8093525
1365.331	0.8129024
1364.331	0.8163688
1363.331	0.8197537
1362.331	0.8230588
1361.331	0.8262861
1360.331	0.8294373
1359.331	0.8325142
1358.331	0.8355186
1357.331	0.8384521
1356.331	0.8413165
1355.331	0.8441132
1354.331	0.8468440
1353.331	0.8495104
1352.331	0.8521139
1351.331	0.8546561
1350.331	0.8571384
1349.331	0.8595622
1348.331	0.8619289
1347.331	0.8642400
1346.331	0.8664968
1345.331	0.8687006
1344.331	0.8708527
1343.331	0.8729544
1342.331	0.8750069
1341.331	0.8770114
1340.331	0.8789691
1339.331	0.8808811
1338.331	0.8827487
1337.331	0.8845728
1336.331	0.8863546
1335.331	0.8880952
1334.331	0.8897955
1333.331	0.8914566
1332.331	0.8930794
1331.331	0.8946650
1330.331	0.8962142
1329.331	0.8977279
1328.331	0.8992071
1327.331	0.9006527
1326.331	0.9020654
1325.331	0.9034461
1324.331	0.9047956
1323.331	0.9061147
1322.331	0.9074042
1321.331	0.9086649
1320.331	0.9098973
1319.331	0.9111023
1318.331	0.9122806
1317.331	0.9134328
1316.331	0.9145596
1315.331	0.9156617
1314.331	0.9167396
1313.331	0.9177939
1312.331	0.9188254
1311.331	0.9198345
1310.331	0.9208217
1309.331	0.9217878
1308.331	0.9227331
1307.331	0.9236583
1306.331	0.9245638
1305.331	0.9254501

```
  1304.331      0.9263177
  1303.331      0.9271671
  1302.331      0.9279988
  1301.331      0.9288131
  1300.331      0.9296105
  1299.331      0.9303915
  1298.331      0.9311564
  1297.363      0.9318915

 PHASE REGION:LIQUID + FCC_A1 + M7C3

    T(C)       fraction solid

  1297.331      0.9321898
  1296.331      0.9644012
  1295.331      0.9850907
  1294.331      0.9951874

Hint: move the last function to the first equilibrium where it is used

  ... the command in full is SET_LABEL_CURVE_OPTION
  ... the command in full is APPEND_EXPERIMENTAL_DATA
```



```
  ... the command in full is APPEND_EXPERIMENTAL_DATA

 ...........................................................

       The following axis variables are available

            T --- Temperature in Celsius
        NL/BL --- Mole/mass fraction of liquid
        NS/BS --- Mole/mass fraction of all solid phases
NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
     W(ph,el) --- Weight fraction of an element in a phase
     X(ph,el) --- Mole fraction of an element in a phase
     Y(ph,el) --- Site fraction of an element in a phase
    NN(ph,el) --- Distribution of an element in a phases
        NH/BH --- Heat release and Latent heat per mole/gram
       CP/BCP --- Apparent heat capacity per mole/gram
    NV/NV(ph) --- Molar volume of the system or a phase
    DS/DS(ph) --- Average density of the system or a phase
           BT --- Apparent volumetric TEC of the system

 "el" and "ph" are name of element and phase, respectively
    "*" can be used as a wild character for "el" and "ph"

 ..........................................................

POST:Hit RETURN to continue
POST: make tcex48a.exp y
  ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
POST: set-dia-ax x ns(fcc_a1)
  ... the command in full is SET_DIAGRAM_AXIS
POST: set-dia-ax y w(fcc_a1,cr)
  ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: plot,,,,,,
  ... the command in full is PLOT_DIAGRAM
```

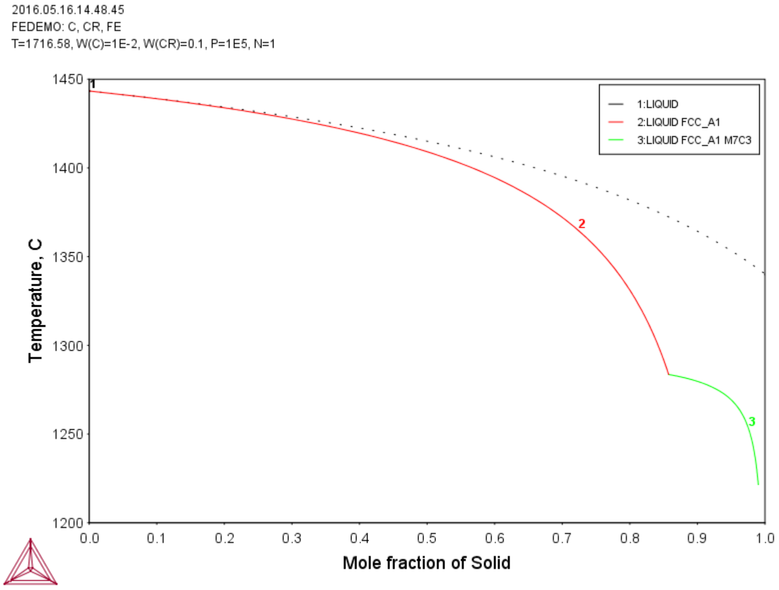


```
POST:Hit RETURN to continue
POST:
POST:
POST: make tcex48b.exp y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
POST: back
SCHEIL: @@
SCHEIL: @@ Ignore back diffusion of C in solids and do Scheil with the same alloy
SCHEIL: @@ by choosing option 3 from the Scheil simulation option list.
SCHEIL: @@ also plot solidification and microsegregation diagrams
SCHEIL: @@ save them to files
SCHEIL: @@
SCHEIL:
SCHEIL: save-file-name tcex48b
SCHEIL: start
   ... the command in full is START_WIZARD
Database /TCFE8/: FEDEMO
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 1
2nd alloying element: cr 10
Next alloying element:
Temperature (C) /2000/: 1700
 VA                        /-  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 CEMENTITE                CHI_A12                  DIAMOND_FCC_A4
 FCC_A1                   GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          M23C6
 M3C2                     M5C2                     M7C3
 SIGMA

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

 ........................................................

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 CEMENTITE                CHI_A12                  DIAMOND_FCC_A4
 FCC_A1                   GRAPHITE                 HCP_A3
 KSI_CARBIDE              LAVES_PHASE_C14          M23C6
 M3C2                     M5C2                     M7C3
 SIGMA

 ........................................................

OK? /Y/: Y
 GAS:G  REJECTED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
```

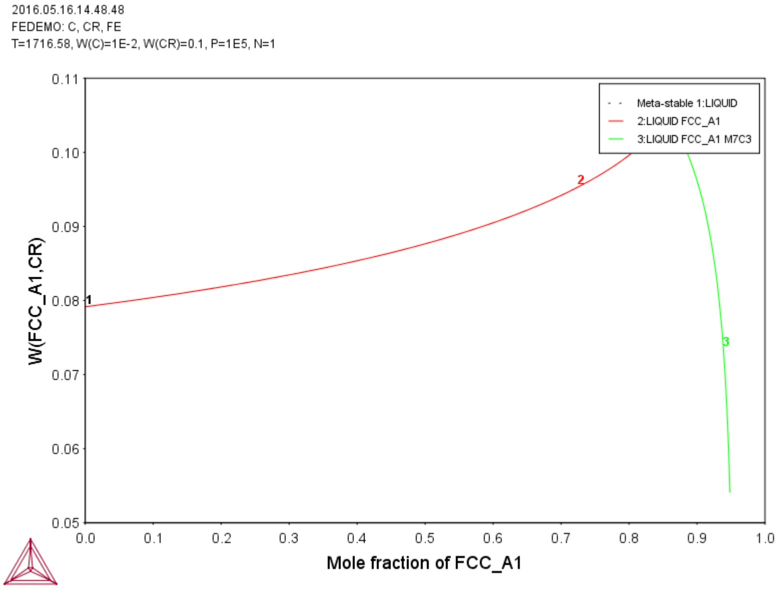
```
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
      data for intermetallic phases. Metals park, Ohio. American Society for
      Metals; Molar volumes'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
      (1986); CR-FE-MO'
  'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, estimated parameter 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
Should any phase have a miscibility gap check? /N/: N
Fast diffusing components: /NONE/: NONE
   ... the command in full is SET_NUMERICAL_LIMITS
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=1973.15, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1    DEGREES OF FREEDOM 0
To form FCC_A1#1 the condition is set to T=1716.48507839
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
   ... the command in full is ADVANCED_OPTIONS
   ... the command in full is STEP_WITH_OPTIONS
...OK

 Phase Region from    1716.48     for:
     LIQUID
     FCC_A1
 Global check of removing phase at  1.71649E+03
 Calculated     3 equilibria

 Phase Region from    1716.49     for:
     LIQUID
 Terminating at    1716.58
 Calculated     4 equilibria

 Phase Region from    1716.48     for:
     LIQUID
     FCC_A1
 Global test at  1.70848E+03 .... OK
 Global test at  1.69848E+03 .... OK
 Global test at  1.68848E+03 .... OK
 Global test at  1.67848E+03 .... OK
 Global test at  1.66848E+03 .... OK
 Global test at  1.65848E+03 .... OK
 Global test at  1.64848E+03 .... OK
 Global test at  1.63848E+03 .... OK
 Global test at  1.62848E+03 .... OK
 Global test at  1.61848E+03 .... OK
 Global check of removing phase at  1.61342E+03
 Calculated   106 equilibria

 Phase Region from    1613.42     for:
     FCC_A1
 Calculated     4 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex48\tcex
 48b.POLY3

  POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

   ... the command in full is ENTER_SYMBOL
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 An EXP file c:\jenkins\WORKSP~1\THERMO~1\examples\tcex48\tcex48b_EQ.EXP
 has been created to store the equilibrium solidification results.
   ... the command in full is READ_WORKSPACES
  CALCULATING SCHEIL SOLIDFICATION
   ... the command in full is SET_NUMERICAL_LIMITS

     T(C)      fraction solid

   1443.425       0.000000

  PHASE REGION:LIQUID + FCC_A1

     T(C)      fraction solid

   1443.331      0.9380064E-04
   1442.331      0.2475714E-01
   1441.331      0.4847007E-01
   1440.331      0.7128104E-01
   1439.331      0.9323546E-01
   1438.331      0.1143759
   1437.331      0.1347424
   1436.331      0.1543724
   1435.331      0.1733012
   1434.331      0.1915621
   1433.331      0.2091864
   1432.331      0.2262034
   1431.331      0.2426409
   1430.331      0.2585253
   1429.331      0.2738811
   1428.331      0.2887318
   1427.331      0.3030994
```

1426.331	0.3170049
1425.331	0.3304680
1424.331	0.3435074
1423.331	0.3561409
1422.331	0.3683853
1421.331	0.3802566
1420.331	0.3917699
1419.331	0.4029396
1418.331	0.4137794
1417.331	0.4243022
1416.331	0.4345205
1415.331	0.4444459
1414.331	0.4540898
1413.331	0.4634626
1412.331	0.4725747
1411.331	0.4814356
1410.331	0.4900547
1409.331	0.4984408
1408.331	0.5066022
1407.331	0.5145470
1406.331	0.5222829
1405.331	0.5298172
1404.331	0.5371570
1403.331	0.5443089
1402.331	0.5512795
1401.331	0.5580748
1400.331	0.5647007
1399.331	0.5711630
1398.331	0.5774669
1397.331	0.5836177
1396.331	0.5896203
1395.331	0.5954796
1394.331	0.6012001
1393.331	0.6067863
1392.331	0.6122422
1391.331	0.6175721
1390.331	0.6227797
1389.331	0.6278689
1388.331	0.6328432
1387.331	0.6377061
1386.331	0.6424610
1385.331	0.6471111
1384.331	0.6516594
1383.331	0.6561089
1382.331	0.6604625
1381.331	0.6647229
1380.331	0.6688929
1379.331	0.6729750
1378.331	0.6769717
1377.331	0.6808852
1376.331	0.6847181
1375.331	0.6884724
1374.331	0.6921504
1373.331	0.6957540
1372.331	0.6992854
1371.331	0.7027464
1370.331	0.7061389
1369.331	0.7094647
1368.331	0.7127256
1367.331	0.7159233
1366.331	0.7190593
1365.331	0.7221353
1364.331	0.7251527
1363.331	0.7281132
1362.331	0.7310181
1361.331	0.7338687
1360.331	0.7366665
1359.331	0.7394127
1358.331	0.7421087
1357.331	0.7447556
1356.331	0.7473545
1355.331	0.7499068
1354.331	0.7524134
1353.331	0.7548755
1352.331	0.7572940
1351.331	0.7596701
1350.331	0.7620047
1349.331	0.7642988
1348.331	0.7665533
1347.331	0.7687690
1346.331	0.7709470
1345.331	0.7730879
1344.331	0.7751928
1343.331	0.7772623
1342.331	0.7792972
1341.331	0.7812983
1340.331	0.7832664
1339.331	0.7852022
1338.331	0.7871063
1337.331	0.7889794
1336.331	0.7908223
1335.331	0.7926355
1334.331	0.7944197
1333.331	0.7961755
1332.331	0.7979034
1331.331	0.7996042
1330.331	0.8012782
1329.331	0.8029261
1328.331	0.8045484
1327.331	0.8061457
1326.331	0.8077183
1325.331	0.8092669
1324.331	0.8107920
1323.331	0.8122939
1322.331	0.8137731
1321.331	0.8152301
1320.331	0.8166654
1319.331	0.8180793
1318.331	0.8194723
1317.331	0.8208447
1316.331	0.8221970
1315.331	0.8235296
1314.331	0.8248428
1313.331	0.8261370
1312.331	0.8274126
1311.331	0.8286698

```
  1310.331      0.8299091
  1309.331      0.8311309
  1308.331      0.8323353
  1307.331      0.8335227
  1306.331      0.8346935
  1305.331      0.8358480
  1304.331      0.8369864
  1303.331      0.8381091
  1302.331      0.8392162
  1301.331      0.8403082
  1300.331      0.8413853
  1299.331      0.8424477
  1298.331      0.8434958
  1297.331      0.8445297
  1296.331      0.8455497
  1295.331      0.8465561
  1294.331      0.8475491
  1293.331      0.8485289
  1292.331      0.8494958
  1291.331      0.8504500
  1290.331      0.8513917
  1289.331      0.8523211
  1288.331      0.8532384
  1287.331      0.8541439
  1286.331      0.8550378
  1285.331      0.8559202
  1284.331      0.8567913
  1283.613      0.8574103

 PHASE REGION:LIQUID + FCC_A1 + M7C3

    T(C)      fraction solid

  1283.581      0.8575876
  1282.581      0.8709413
  1281.581      0.8824023
  1280.581      0.8923216
  1279.581      0.9009710
  1278.581      0.9085643
  1277.581      0.9152712
  1276.581      0.9212283
  1275.581      0.9265464
  1274.581      0.9313162
  1273.581      0.9356128
  1272.581      0.9394983
  1271.581      0.9430252
  1270.581      0.9462374
  1269.581      0.9491724
  1268.581      0.9518620
  1267.581      0.9543337
  1266.581      0.9566111
  1265.581      0.9587145
  1264.581      0.9606618
  1263.581      0.9624685
  1262.581      0.9641482
  1261.581      0.9657129
  1260.581      0.9671731
  1259.581      0.9685382
  1258.581      0.9698165
  1257.581      0.9710154
  1256.581      0.9721416
  1255.581      0.9732011
  1254.581      0.9741990
  1253.581      0.9751403
  1252.581      0.9760293
  1251.581      0.9768699
  1250.581      0.9776656
  1249.581      0.9784196
  1248.581      0.9791350
  1247.581      0.9798144
  1246.581      0.9804603
  1245.581      0.9810748
  1244.581      0.9816600
  1243.581      0.9822179
  1242.581      0.9827501
  1241.581      0.9832582
  1240.581      0.9837437
  1239.581      0.9842081
  1238.581      0.9846524
  1237.581      0.9850780
  1236.581      0.9854858
  1235.581      0.9858768
  1234.581      0.9862521
  1233.581      0.9866124
  1232.581      0.9869586
  1231.581      0.9872915
  1230.581      0.9876116
  1229.581      0.9879197
  1228.581      0.9882164
  1227.581      0.9885023
  1226.581      0.9887779
  1225.581      0.9890437
  1224.581      0.9893001
  1223.581      0.9895477
  1222.581      0.9897868
  1221.581      0.9900178

Hint: move the last function to the first equilibrium where it is used

  ... the command in full is SET_LABEL_CURVE_OPTION
  ... the command in full is APPEND_EXPERIMENTAL_DATA
```

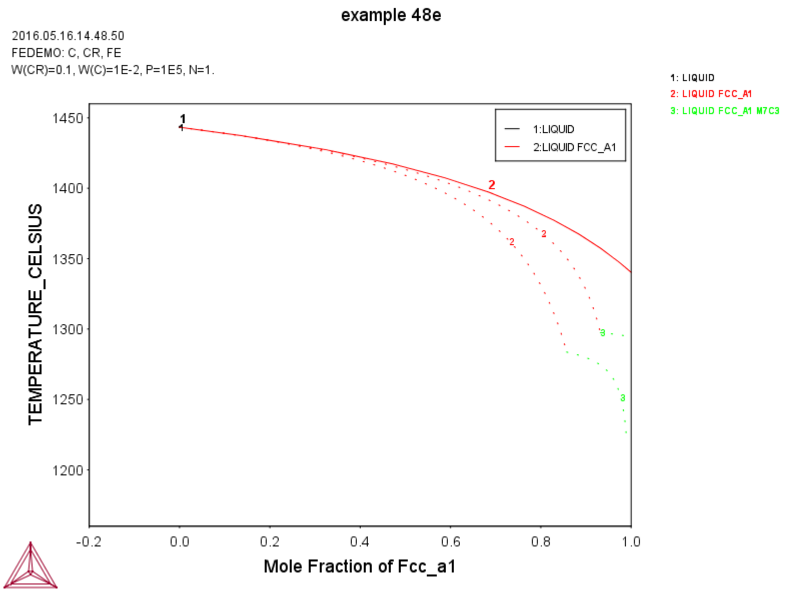


```
   ... the command in full is APPEND_EXPERIMENTAL_DATA

  ............................................................

        The following axis variables are available

             T --- Temperature in Celsius
         NL/BL --- Mole/mass fraction of liquid
         NS/BS --- Mole/mass fraction of all solid phases
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
      W(ph,el) --- Weight fraction of an element in a phase
      X(ph,el) --- Mole fraction of an element in a phase
      Y(ph,el) --- Site fraction of an element in a phase
     NN(ph,el) --- Distribution of an element in a phases
         NH/BH --- Heat release and Latent heat per mole/gram
        CP/BCP --- Apparent heat capacity per mole/gram
     NV/NV(ph) --- Molar volume of the system or a phase
     DS/DS(ph) --- Average density of the system or a phase
            BT --- Apparent volumetric TEC of the system

  "el" and "ph" are name of element and phase, respectively
     "*" can be used as a wild character for "el" and "ph"

  ...........................................................

POST:Hit RETURN to continue
POST: make tcex48c.exp y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: set-dia-ax x ns(fcc_a1)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-dia-ax y w(fcc_a1,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: plot,,,,,
   ... the command in full is PLOT_DIAGRAM
```

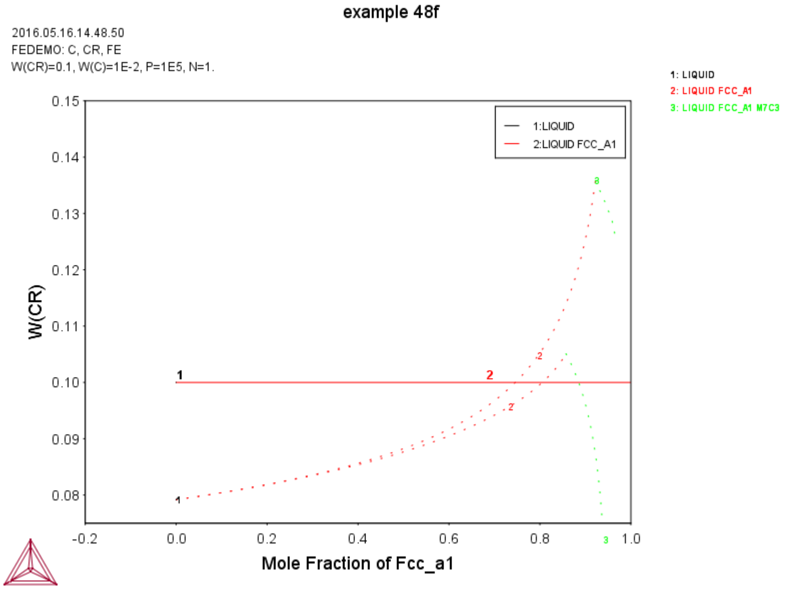


```
POST: make tcex48d.exp y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
SCHEIL:Hit RETURN to continue
SCHEIL: @@ calculate simple equilibrium solidification of the same alloy
SCHEIL: @@ and compare the results with those of Scheil and ScheiC
SCHEIL: go p-3
   ... the command in full is GOTO_MODULE
POLY_3: read tcex48b
   ... the command in full is READ_WORKSPACES
POLY_3: list-condition
   ... the command in full is LIST_CONDITIONS
 T=1716.58, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1
 DEGREES OF FREEDOM 0
```

```
POLY_3: list-equilibrium
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: FEDEMO

 Conditions:
 T=1716.58, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1716.58 K (  1443.43 C),  Pressure  1.000000E+05
 Number of moles of components  1.02132E-02,  Mass in grams  4.94687E-01
 Total Gibbs energy -9.92311E+02,  Enthalpy  6.48245E+02,  Volume  7.34133E-08

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        1.6474E-03  3.9998E-02 4.6838E-02 -4.3689E+04 SER
 CR                       9.0314E-04  9.4928E-02 2.0203E-04 -1.2142E+05 SER
 FE                       7.6627E-03  8.6507E-01 1.3719E-03 -9.4078E+04 SER

 LIQUID                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.7543E-03, Mass 4.7227E-01, Volume fraction 9.5694E-01  Mass fractions:
 FE  8.66714E-01  CR  9.31259E-02  C   4.01602E-02

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
 Moles 3.1121E-04, Mass 1.6266E-02, Volume fraction 3.1001E-02  Mass fractions:
 FE  9.28665E-01  CR  5.36480E-02  C   1.76870E-02

 M7C3                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.4776E-04, Mass 6.1527E-03, Volume fraction 1.2058E-02  Mass fractions:
 FE  5.71093E-01  CR  3.42373E-01  C   8.65339E-02
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: reinit
   ... the command in full is REINITIATE_MODULE
POLY_3: set-condition t=1717.15 w(cr)=0.1 w(c)=0.01 p=1e5 n=1
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    31 ITS,  CPU TIME USED   0 SECONDS
POLY_3: set-ax-var 1 t 500 1717.15 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: break-condition
Break condition: np(liquid)=0
POLY_3: save tcex48c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, trying to add one                      0
 Step will start from axis value    1717.15

 Phase Region from    1717.15     for:
     LIQUID
 Calculated     4 equilibria

 Phase Region from    1716.48     for:
     LIQUID
     FCC_A1
 Calculated    13 equilibria

 Phase Region from    1613.42     for:
     FCC_A1
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex48\tcex
 48c.POLY3
POLY_3: post
POST: @@ define a function to get amount of solids
POST: ent fun fs=1-np(liquid);
   ... the command in full is ENTER_SYMBOL
POST: @@ plot solidification diagram
POST: set-dia-ax x fs
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-dia-ax y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: append-exp y tcex48a tcex48c 0; 1; 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-ax-text x n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Mole Fraction of Fcc_a1
POST: set-scaling-status y n 1160 1460
POST: set-title example 48e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: @@ plot microsegregation which represent the composition profile
POST: @@ of the solid. For equilibrium solidification
POST: @@ there is no solute segregation and the composition of
POST: @@ solidified solid is uniform.
POST: set-dia-ax x fs
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-dia-ax y w(cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: append-exp y tcex48b tcex48d 0; 1; 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-ax-text x n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Mole Fraction of Fcc_a1
POST: set-scaling y n 0.075 0.15
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 48f
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

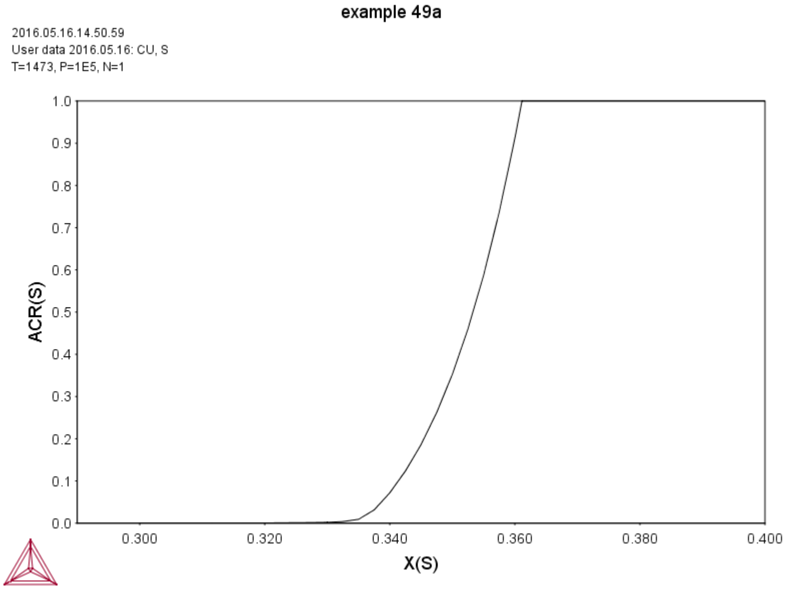
tcex49

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex49\tcex49.TCM" set-echo
SYS: @@
SYS: @@ Quasichemical Model via GES
SYS: @@
SYS: @@ Example showing entering parameter for FACT quasichemical liquid model
SYS: @@ and calculating the sulfur activity
SYS:
SYS: set-log ex49,,,
SYS:
SYS:  go gibbs
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES:  ent-el  /- VA CU S
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
GES:  am_el_d /-  ELECTRON_GAS      0.0000E+00  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES:  am_el_d VA  VACUUM            0.0000E+00  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES:  am_el_d CU  FCC_A1            6.3546E+01  5.0041E+03  3.3150E+01 1
   ... the command in full is AMEND_ELEMENT_DATA
GES:  am_el_d S   FC_ORTHORHOMBIC   3.2066E+01  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES:
GES:
GES: @@ The quasichemical model requires species entered with the
GES: @@ stoichiometry.  The factor 2/ZZ is needed
GES: @@ for the pure elements and 1/ZZ for the compounds.
GES: @@ For Cu ZZ=0.9294 and 2/ZZ_Cu=2.15193
GES: @@ For S  ZZ=1.8366 and 2/ZZ_S=1.08897
GES: @@ For CuS the stoichiometries are thus 1/ZZ_Cu=1.07596 and
GES: @@ 1/ZZ_S=0.54448
GES:
GES:  enter-specie CUQ                        CU2.15193
   ... the command in full is ENTER_SPECIES
GES:  enter-specie CUQS                       CU1.07596S0.54448
   ... the command in full is ENTER_SPECIES
GES:  enter-specie S2                         S2
   ... the command in full is ENTER_SPECIES
GES:  enter-specie SQ                         S1.08897
   ... the command in full is ENTER_SPECIES
GES:
GES:
GES: @@ The Gibbs energy difference between FCC-Cu and quasichemical liquid-Cu
GES:
GES:  ent-sym fun GQCU  2.98150E+02  +16547-7.6815*T;    6.00000E+03   N
   ... the command in full is ENTER_SYMBOL
GES:
GES:
GES: @@ The Gibbs energy difference between GAS-S and quasichemical liquid-S
GES:
GES:  ent-sym fun GQS   2.98150E+02  -65357+165.396*T-13.513*T*LN(T);
   ... the command in full is ENTER_SYMBOL
HIGH TEMPERATURE LIMIT /6000/:      6.00000E+03   N
GES:
GES:
GES:
GES: @@ Gibbs energies for the pure elements and gases refered to SER
GES:  ent-sym fun GHSERCU   2.98150E+02  -7770.458+130.485403*T
   ... the command in full is ENTER_SYMBOL
&      -24.112392*T*LN(T)-.00265684*T**2+1.29223E
&      -07*T**3+52478*T**(-1);  1.35802E+03  Y
FUNCTION:       -13542.33+183.804197*T-31.38*T*LN(T)+3.64643E+29*T**(-9);
HIGH TEMPERATURE LIMIT /6000/:      3.20000E+03 N
GES:  ent-sym fun GS2GAS    2.98150E+02  +117374.548+2.98629558*T
   ... the command in full is ENTER_SYMBOL
&      -34.09678*T*LN(T)-.002325464*T**2+1.85480167E-07*T**3
&      +128593.6*T**(-1);  1.00000E+03  Y
FUNCTION:       +117352.438+2.50383258*T-34.04744*T*LN(T)-.0021150245*T**2
&      +9.16602333E-08*T**3+175718.45*T**(-1);  3.40000E+03  Y
FUNCTION:       +124361.091+14.5182895*T-36.1923*T*LN(T)-5.930925E-04*T**2
&      -7.54259333E-09*T**3-7484105*T**(-1);  6.00000E+03  N
GES:  ent-sym fun GSSLIQ    2.98150E+02  -4001.549+77.889686*T
   ... the command in full is ENTER_SYMBOL
&      -15.504*T*LN(T)-.018629*T**2-2.4942E-07*T**3
&      -113945*T**(-1);  3.88360E+02  Y
FUNCTION:       -5285183.35+118449.585*T-19762.4*T*LN(T)+32.79275*T**2
&      -.0102214167*T**3+2.646735E+08*T**(-1);  4.28150E+02  Y
FUNCTION:       -8174995.23+319914.078*T-57607.3*T*LN(T)+135.3045*T**2
&      -.0529973333*T**3;  4.32250E+02  Y
FUNCTION:       -219408.801+7758.83993*T-1371.85*T*LN(T)+2.845035*T**2
&      -.00101380333*T**3;  4.53150E+02  Y
FUNCTION:       +92539.872-1336.36627*T+202.958*T*LN(T)-.2531915*T**2
&      +5.18835E-05*T**3-8202200*T**(-1);  7.17000E+02  Y
FUNCTION:        -6889.972+176.35482*T-32*T*LN(T);  1.30000E+03  N
GES:  ent-sym fun GCULIQ    2.98150E+02  +12964.84-9.510243*T
   ... the command in full is ENTER_SYMBOL
&      -5.83932E-21*T**7+GHSERCU ;  1.35802E+03  Y
FUNCTION:        +13495.4-9.920463*T-3.64643E+29*T**(-9)+GHSERCU ;
HIGH TEMPERATURE LIMIT /6000/:       3.20000E+03  N
GES:
GES:
GES:
GES:  ent-phase GAS  G,  1   S2 ;  N N
   ... the command in full is ENTER_PHASE
GES:
GES:
GES:  ent-param G(GAS,S2;0)  2.98150E+02  +GS2GAS +RTLNP ;
   ... the command in full is ENTER_PARAMETER
 G(GAS,S2;0)- 2 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/:         6.00000E+03   N
GES:
GES:
```

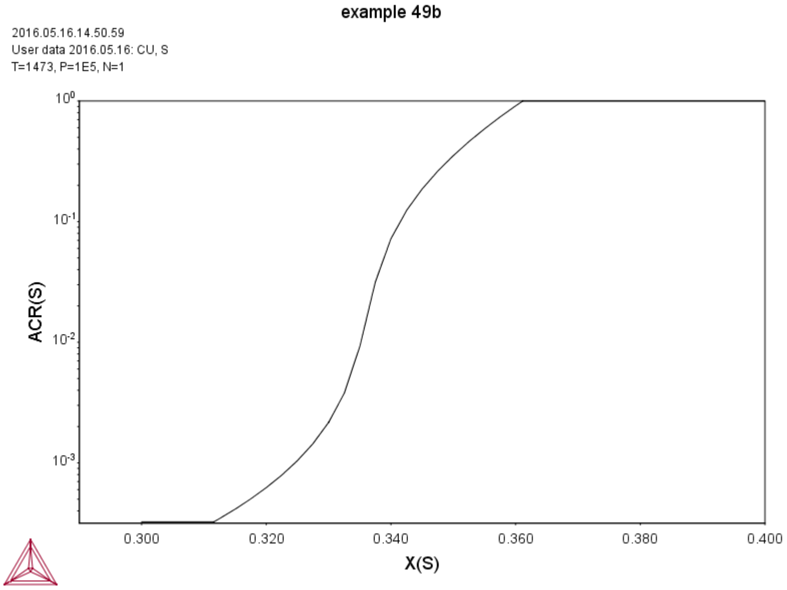
```
GES:
GES:  ent-phase FCC_A1  ,  1   CU ;  N N
   ... the command in full is ENTER_PHASE
GES:  amend_phase FCC_A1 magnetic  -3.0    2.80000E-01
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES:
GES:  ent-param G(FCC_A1,CU;0) 2.98150E+02 +GHSERCU; 3.20000E+03  N
   ... the command in full is ENTER_PARAMETER
 G(FCC_A1,CU;0)-G(FCC_A1,CU;0)
GES:
GES:
GES:
GES:  ent-phase QUASI  L,  1    CUQ,CUQS,SQ ;  N N
   ... the command in full is ENTER_PHASE
GES:
GES:
GES: @@ The stoichiometry parameter for pure Cu is 2/ZZ,
GES: @@ the stoichiometry ratio
GES:
GES:  ent-param VK(QUASI,CUQ;0)  2.98150E+02 .9294; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 VK(QUASI,CUQ;0)
GES:
GES: @@ The energy parameter for pure Cu (factor is 2/VK)
GES:
GES:  ent-param G(QUASI,CUQ;0)  2.98150E+02  +2.15193*GCULIQ
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ;0)-2.15193 G(FCC_A1,CU;0)
&       +2.15193*GQCU ;   6.00000E+03   N
GES:
GES: @@ The Gibbs energy parameter for the molecule CUQS
GES: @@ (factors 1/ZZ_cu and 1/ZZ_s)
GES:
GES:  ent-param G(QUASI,CUQS;0)  2.98150E+02  +1.07596*GCULIQ
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQS;0)-1.07596 G(FCC_A1,CU;0)-0.54448 G(FC_ORTHORHOMBIC,S;0)
&       +1.075963*GQCU+.54448*GSSLIQ ;  6.00000E+03   N
GES:
GES:
GES: @@ The stoichiometry parameter for pure S is 2/ZZ
GES:
GES:  ent-param VK(QUASI,SQ;0) 2.98150E+02 1.8366; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 VK(QUASI,SQ;0)
GES:
GES: @@ The energy parameter for pure S (factor is 2/VK)
GES:
GES:  ent-param G(QUASI,SQ;0)  2.98150E+02  +1.08897*GSSLIQ ;
   ... the command in full is ENTER_PARAMETER
 G(QUASI,SQ;0)-1.08897 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/:         6.00000E+03   N
GES:
GES: @@ The mixing terms
GES:
GES:  ent-param G(QUASI,CUQ,CUQS;0) 2.98150E+02  -82768; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;0)
GES:  ent-param G(QUASI,CUQ,CUQS;1) 2.98150E+02  -32070; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;1)
GES:  ent-param G(QUASI,CUQ,CUQS;2) 2.98150E+02  68734; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;2)
GES:  ent-param G(QUASI,CUQ,CUQS;3) 2.98150E+02  -84194+50*T;
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;3)
HIGH TEMPERATURE LIMIT /6000/:     6.00000E+03   N
GES:  ent-param G(QUASI,CUQ,CUQS;4) 2.98150E+02  -43638; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;4)
GES:  ent-param G(QUASI,CUQ,CUQS;5) 2.98150E+02  +20*T;  6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;5)
GES:
GES:
GES: @@ This command makes the entropy calculation according to
GES: @@ FACT quasichemical model
GES:
GES: amend-phase-description QUASI quasi-fact00
GES:
GES: @@ Binary excess Legendre with 1 as independent
GES: @@ Note that the order of the species are important!
GES:
GES: amend-phase-description QUASI excess
MODEL NAME /REDLICH-KISTER_MUGGIANU/: mixed
First (the independent) constituent: CUQ
Second (the dependent) constituent: CUQS
Excess model type: /LEGENDRE/: Legendre

 Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent: NONE
GES:
GES:
GES:
GES: list-data
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE: User data 2016.05.16

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 CU   FCC_A1                    6.3546E+01  5.0041E+03  3.3150E+01
  2 S    FC_ORTHORHOMBIC           3.2066E+01  0.0000E+00  0.0000E+00
```

```
 SPECIES                                    STOICHIOMETRY
   1 CU                                     CU
   2 CUQ                                    CU2.15193
   3 CUQS                                   CU1.07596S0.54448
   4 S                                      S
   5 S2                                     S2
   6 SQ                                     S1.08897
   7 VA                                     VA



 GAS
    CONSTITUENTS: S2

      G(GAS,S2;0)- 2 G(FC_ORTHORHOMBIC,S;0) = +GS2GAS+RTLNP


 QUASI
 $ QUASICHEMICAL-FACT00 ENTROPY CONTRIBUTION
    CONSTITUENTS: CUQ,CUQS,SQ

      VK(QUASI,CUQ;0) = +.9294
      G(QUASI,CUQ;0)-2.15193 G(FCC_A1,CU;0) = +2.15193*GCULIQ+2.15193*GQCU
      G(QUASI,CUQS;0)-1.07596 G(FCC_A1,CU;0)-0.54448 G(FC_ORTHORHOMBIC,S;0) =
            +1.07596*GCULIQ+1.075963*GQCU+.54448*GSSLIQ
      VK(QUASI,SQ;0) = +1.8366
      G(QUASI,SQ;0)-1.08897 G(FC_ORTHORHOMBIC,S;0) = +1.08897*GSSLIQ
$ Binary excess model Legendre with CUQ as independent
      L(QUASI,CUQ,CUQS;0) = -82768
      L(QUASI,CUQ,CUQS;1) = -32070
      L(QUASI,CUQ,CUQS;2) = +68734
      L(QUASI,CUQ,CUQS;3) = -84194+50*T
      L(QUASI,CUQ,CUQS;4) = -43638
      L(QUASI,CUQ,CUQS;5) = +20*T


 FCC_A1
 ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
      Magnetic function below Curie Temperature
      +1-.860338755*TAO**(-1)-.17449124*TAO**3-.00775516624*TAO**9
      -.0017449124*TAO**15
      Magnetic function above Curie Temperature
       -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)
      -2.84601512E-04*TAO**(-25)
    CONSTITUENTS: CU

      G(FCC_A1,CU;0)-G(FCC_A1,CU;0) =    298.15<T< 3200.00: +GHSERCU

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 103 GQCU      20000000 +16547-7.6815*T
 104 GQS       20000000 -65357+165.396*T-13.513*T*LN(T)
 105 GHSERCU   20000000
       298.15<T< 1358.02: -7770.458+130.485403*T-24.112392*T*LN(T)
     -.00265684*T**2+1.29223E-07*T**3+52478*T**(-1)
      1358.02<T< 3200.00: -13542.33+183.804197*T-31.38*T*LN(T)
     +3.64643E+29*T**(-9)
 106 GS2GAS    20000000
       298.15<T< 1000.00: +117374.548+2.98629558*T-34.09678*T*LN(T)
     -.002325464*T**2+1.85480167E-07*T**3+128593.6*T**(-1)
      1000.00<T< 3400.00: +117352.438+2.50383258*T-34.04744*T*LN(T)
     -.0021150245*T**2+9.16602333E-08*T**3+175718.45*T**(-1)
      3400.00<T< 6000.00: +124361.091+14.5182895*T-36.1923*T*LN(T)
     -5.930925E-04*T**2-7.54259333E-09*T**3-7484105*T**(-1)
 107 GSSLIQ    20000000
       298.15<T<  388.36: -4001.549+77.889686*T-15.504*T*LN(T)-.018629*T**2
     -2.4942E-07*T**3-113945*T**(-1)
       388.36<T<  428.15: -5285183.35+118449.585*T-19762.4*T*LN(T)
     +32.79275*T**2-.0102214167*T**3+2.646735E+08*T**(-1)
       428.15<T<  432.25: -8174995.23+319914.078*T-57607.3*T*LN(T)
     +135.3045*T**2-.0529973333*T**3
       432.25<T<  453.15: -219408.801+7758.83993*T-1371.85*T*LN(T)
     +2.845035*T**2-.00101380333*T**3
       453.15<T<  717.00: +92539.872-1336.36627*T+202.958*T*LN(T)
     -.2531915*T**2+5.18835E-05*T**3-8202200*T**(-1)
       717.00<T< 1300.00: -6889.972+176.35482*T-32*T*LN(T)
 108 GCULIQ    20000000
       298.15<T< 1358.02: +12964.84-9.510243*T-5.83932E-21*T**7+GHSERCU
      1358.02<T< 3200.00: +13495.4-9.920463*T-3.64643E+29*T**(-9)+GHSERCU


GES:
GES:Hit RETURN to continue
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3:
POLY_3:
POLY_3:
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FCC_A1                  ENTERED      0.000000E+00    0.000000E+00
 QUASI                   ENTERED      0.000000E+00    0.000000E+00
 GAS                     ENTERED      0.000000E+00    0.000000E+00
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p q gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: ENTERED
Start value, number of moles /0/: 0
POLY_3:
POLY_3:
POLY_3: s-c t=1473 p=1e5 n=1 x(s)=.33
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1978 grid points in              0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
```

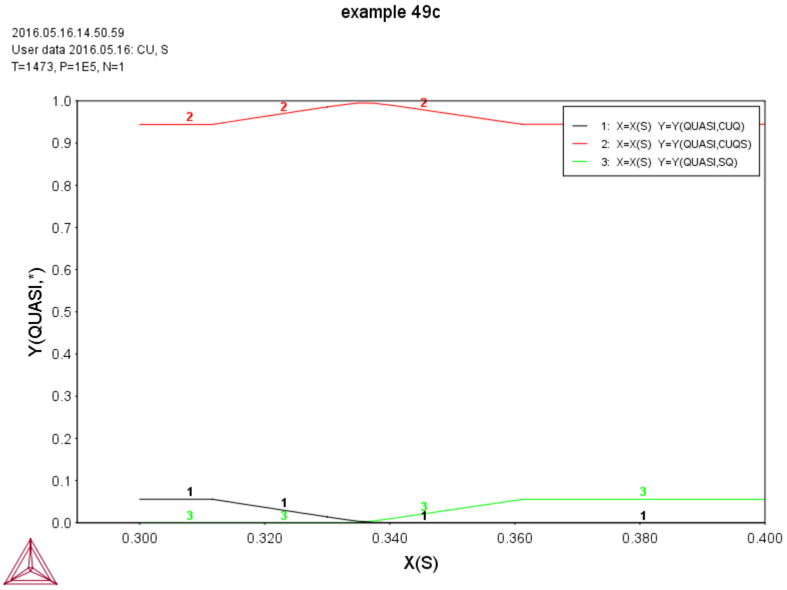
```
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=1473, P=1E5, N=1, X(S)=0.33
 DEGREES OF FREEDOM 0

 Temperature   1473.00 K (  1199.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.31576E+01
 Total Gibbs energy -1.24169E+05,  Enthalpy  1.52783E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CU                      6.7000E-01  8.0094E-01 8.2231E-04 -8.6997E+04 SER
 S                       3.3000E-01  1.9906E-01 8.3318E-08 -1.9964E+05 SER

 QUASI                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3158E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  8.00936E-01  S   1.99064E-01
POLY_3:Hit RETURN to continue
POLY_3: s-r-s s gas
   ... the command in full is SET_REFERENCE_STATE
Temperature /*/: *
Pressure /1E5/: 1E5
POLY_3: sh acr(s)
   ... the command in full is SHOW_VALUE
 ACR(S)=2.1652884E-3
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 x(s)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: .3
Max value /1/: .4
Increment /.0025/: .0025
POLY_3: save tcex49 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.330000
...OK

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.61133E-01
 Calculated    15 equilibria

 Phase Region from   0.361133     for:
     GAS
     QUASI
 Global test at  3.80000E-01 .... OK
 Terminating at   0.400000
 Calculated    19 equilibria

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.10000E-01 .. Creating a new composition set QUASI#2
 Backtracking to find phase change for QUASI#2
 Global test at  3.27500E-01 .... OK
 Global test at  3.22500E-01 .... OK
 Global test at  3.17500E-01 .... OK
 Global test at  3.12500E-01 .... OK
 Global check of adding phase at  3.11581E-01
 Calculated    11 equilibria

 Phase Region from   0.311581     for:
     QUASI
     QUASI#2
 Terminating at   0.300000
 Calculated     8 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex49\tcex
 49.POLY3
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y acr(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: set-title example 49b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

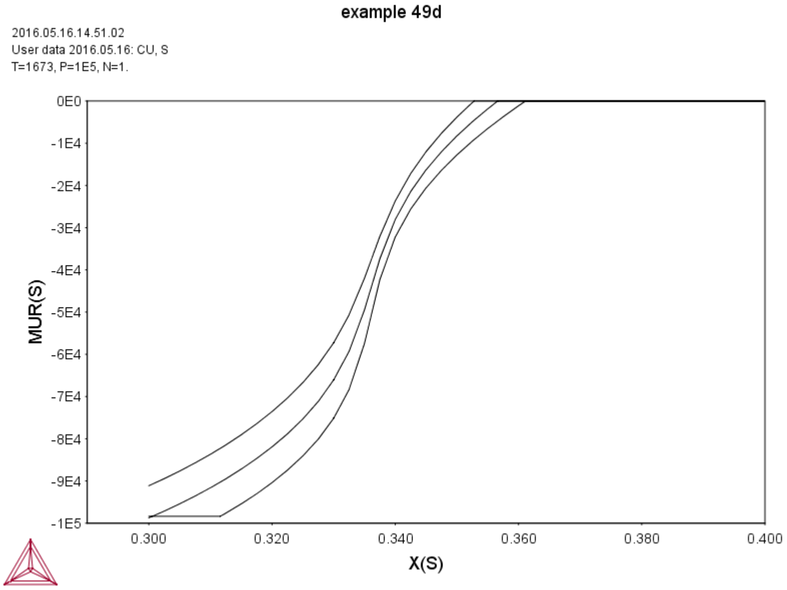


```
POST:
POST:Hit RETURN to continue
POST: s-d-a y y(quasi,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: s-a-ty y lin
   ... the command in full is SET_AXIS_TYPE
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 49c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:
POST:@?
POST: back
POLY_3: read tcex49
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-c t=1573
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1978 grid points in               0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       0 s, total time      0  s
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.330000
...OK

 Phase Region from   0.330000      for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.56605E-01
 Calculated    13 equilibria

 Phase Region from   0.356605      for:
     GAS
     QUASI
 Global test at  3.75000E-01 .... OK
 Global test at  4.00000E-01 .... OK
 Terminating at   0.400000
 Calculated    21 equilibria

 Phase Region from   0.330000      for:
     QUASI
 Global test at  3.10000E-01 .... OK
 Terminating at   0.300000
 Calculated    15 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex49\tcex
 49.POLY3
POLY_3:
POLY_3: read tcex49
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-c t=1673
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1978 grid points in               1 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       0 s, total time      1  s
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.330000
...OK

 Phase Region from   0.330000      for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.52789E-01
 Calculated    12 equilibria

 Phase Region from   0.352789      for:
     GAS
     QUASI
 Global test at  3.72500E-01 .... OK
 Global test at  3.97500E-01 .... OK
 Terminating at   0.400000
 Calculated    22 equilibria

 Phase Region from   0.330000      for:
     QUASI
 Global test at  3.10000E-01 .... OK
 Terminating at   0.300000
 Calculated    15 equilibria
```

```
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex49\tcex
 49.POLY3
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a y mur(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



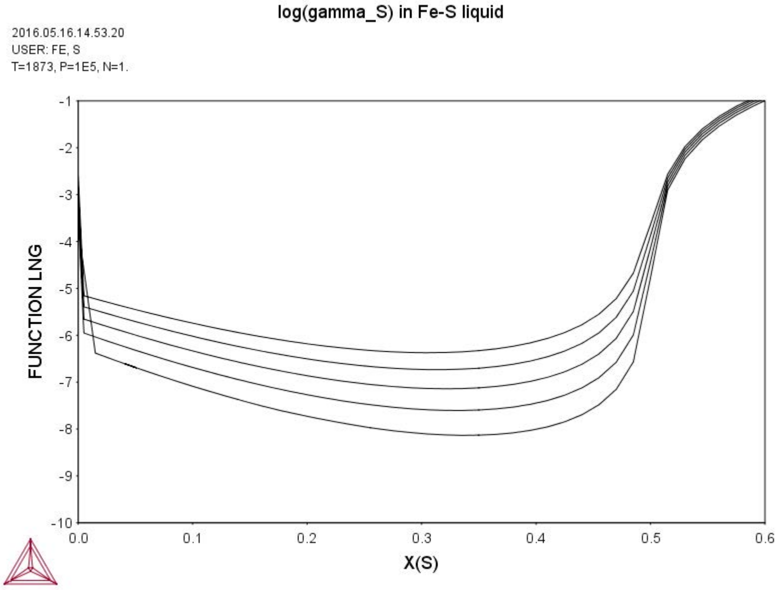
```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex50

```
About Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex50\tcex50.TCM" set-echo
SYS: @@
SYS: @@ Quasichemical Model via TDB
SYS: @@
SYS: @@ Calculation of Fig 3+4 in Kongoli et al
SYS: @@ Metall. Mater. Trans. B, 29B(1998)591.
SYS: @@ Fe-S
SYS:
SYS: set-log ex50,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw user tcex50
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

TDB_USER: d-sys fe s
   ... the command in full is DEFINE_SYSTEM
 FE                       S  DEFINED
TDB_USER: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE lattice stabilities, Calphad 1991'
  'Kongoli, Dessureault and Pelton, Met Trans B, 29B (1998) p 591-601'
 AFTER ...
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p quasi=ent 1
   ... the command in full is CHANGE_STATUS
POLY_3: s-r-s s quasi * 1E5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: enter fun lng=log(acr(s)/x(s));
   ... the command in full is ENTER_SYMBOL
POLY_3: s-c t=1573 p=1e5 n=1 x(s)=.35
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: s-a-v 1 x(s) 0 .6,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: s-c t=1473
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1573
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1673
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1773
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
```

```
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1873
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: save tcex50 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
...OK
...OK
...OK
...OK
...OK

 Phase Region from   0.350000     for:
     QUASI
 Global test at  4.70000E-01 .... OK
 Terminating at   0.600000
 Calculated    20 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  2.30000E-01 .. Creating a new composition set QUASI#2
 Backtracking to find phase change for QUASI#2
 Global test at  3.35000E-01 .... OK
 Global test at  3.05000E-01 .... OK
 Global test at  2.75000E-01 .... OK
 Global test at  2.57000E-01 .... OK
 Global check of adding phase at  2.55243E-01
 Calculated    11 equilibria

 Phase Region from   0.255243     for:
     QUASI
     QUASI#2
 Global test at  1.46000E-01 .... OK
 Global check of removing phase at  1.39331E-01
 Calculated    11 equilibria

 Phase Region from   0.139331     for:
     QUASI#2
 Global test at  2.60000E-02 .... OK
 Backtracking to find phase change for QUASI#1
 Global test at  1.31000E-01 .... OK
 Global test at  1.01000E-01 .... OK
 Global test at  7.10000E-02 .... OK
 Global test at  4.10000E-02 .... OK
 Global test at  1.10000E-02 .... OK
 Backtracking to find phase change for QUASI#1
 Global check of adding phase at  5.03828E-02
 Calculated    11 equilibria

 Phase Region from   0.503828E-01 for:
     QUASI
     QUASI#2
 Global check of removing phase at  5.03830E-02
 Calculated     3 equilibria

 Phase Region from   0.503830E-01 for:
     QUASI#2
 Terminating at   0.127672E-10
 Calculated     7 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  4.70000E-01 .... OK
 Terminating at   0.600000
 Calculated    20 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  2.30000E-01 .... OK
 Global test at  8.00000E-02 .... OK
 Terminating at   0.125999E-10
 Calculated    27 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  4.70000E-01 .... OK
 Terminating at   0.600000
 Calculated    20 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  2.30000E-01 .... OK
 Global test at  8.00000E-02 .... OK
 Terminating at   0.124527E-10
 Calculated    27 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  4.70000E-01 .... OK
 Terminating at   0.600000
 Calculated    20 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  2.30000E-01 .... OK
 Global test at  8.00000E-02 .... OK
 Terminating at   0.123222E-10
 Calculated    27 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  4.70000E-01 .... OK
 Terminating at   0.600000
 Calculated    20 equilibria

 Phase Region from   0.350000     for:
```

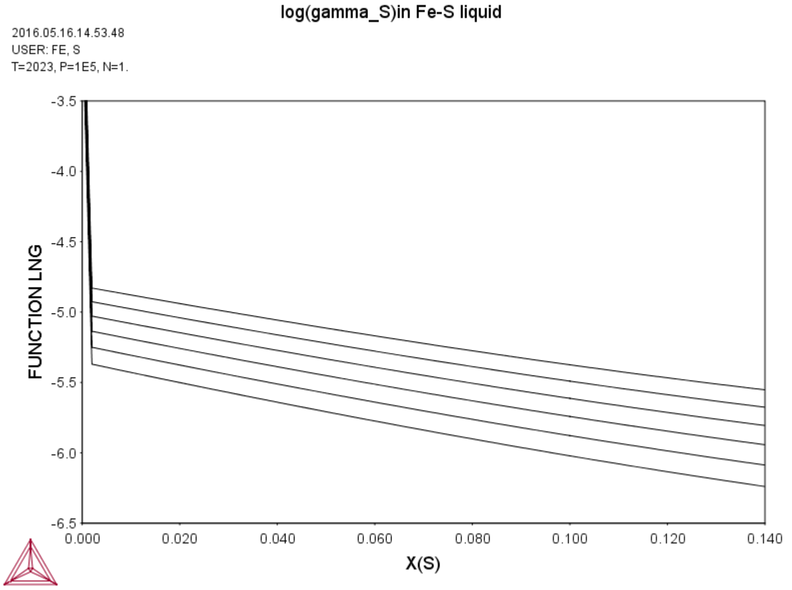
```
    QUASI
 Global test at  2.30000E-01 .... OK
 Global test at  8.00000E-02 .... OK
 Terminating at   0.122058E-10
 Calculated    27 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex50\tcex
 50.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y lng
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n -10 -1
   ... the command in full is SET_SCALING_STATUS
POST: set-title log(gamma_S) in Fe-S liquid
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: back
POLY_3: read tcex50
   ... the command in full is READ_WORKSPACES
POLY_3: rei
   ... the command in full is REINITIATE_MODULE
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p quasi=ent 1
   ... the command in full is CHANGE_STATUS
POLY_3: s-r-s s quasi * 1E5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: enter fun lng=log(acr(s)/x(s));
   ... the command in full is ENTER_SYMBOL
POLY_3: s-c t=1773 p=1e5 n=1 x(s)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex50 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: s-a-v 1 x(s) 0 .14 ,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1823
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1873
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1923
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
```

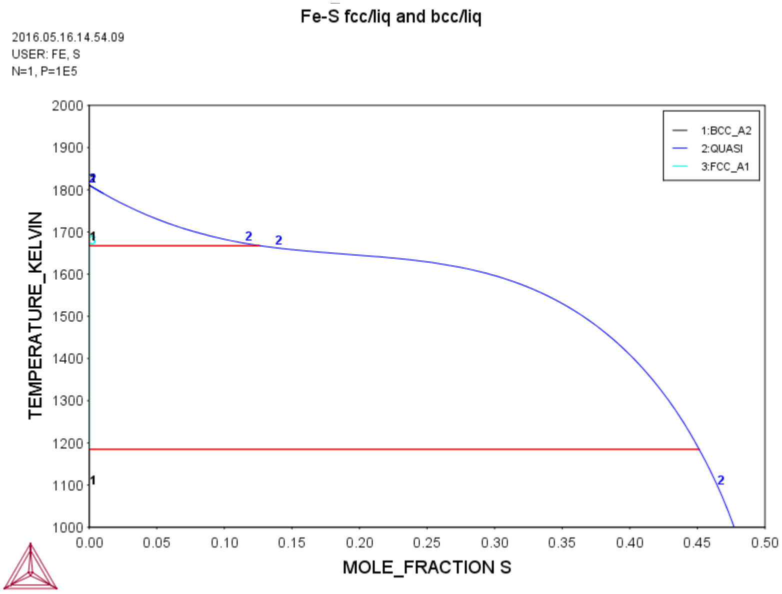
```
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1973
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=2023
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
...OK
...OK
...OK
...OK
...OK
...OK

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.123099E-10
 Calculated    32 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.122501E-10
 Calculated    32 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.121935E-10
 Calculated    32 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.121398E-10
 Calculated    32 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.120889E-10
 Calculated    32 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000E+00 for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.120406E-10
```

```
 Calculated    32 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex50\tcex
 50.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y lng
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 0 .14
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n -6.5 -3.5
   ... the command in full is SET_SCALING_STATUS
POST: set-title log(gamma_S)in Fe-S liquid
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: back
POLY_3: read tcex50
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: rei
   ... the command in full is REINITIATE_MODULE
POLY_3: s-c x(s)=.01 t=1900 n=1 p=1e5
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           1981 grid points in              0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0   , database: USER

 Conditions:
 X(S)=1E-2, T=1900, N=1, P=1E5
 DEGREES OF FREEDOM 0

 Temperature   1900.00 K (  1626.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.56092E+01
 Total Gibbs energy -1.19028E+05,  Enthalpy  7.56841E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 FE                       9.9000E-01  9.9423E-01 5.9397E-04 -1.1736E+05 SER
 S                        1.0000E-02  5.7663E-03 5.9092E-05 -1.5381E+05 QUASI

 QUASI                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.5609E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.94234E-01  S   5.76631E-03
POLY_3:Hit RETURN to continue
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1200
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           1981 grid points in              0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-a-v 1 x(s) 0 .5 0.01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1000 2000 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex50 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
```

```
 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4

 Phase region boundary   1 at:   5.000E-03  1.792E+03
  ** BCC_A2
     QUASI
 Calculated                      15  equilibria

 Phase region boundary   2 at:   5.000E-03  1.792E+03
  ** BCC_A2
     QUASI
 Calculated.                      21  equilibria

 Phase region boundary   3 at:   6.305E-02  1.667E+03
  ** BCC_A2
  ** FCC_A1
     QUASI

 Phase region boundary   4 at:   6.305E-02  1.667E+03
  ** FCC_A1
     QUASI
 Calculated.                     162  equilibria

 Phase region boundary   5 at:   2.256E-01  1.185E+03
  ** BCC_A2
  ** FCC_A1
     QUASI

 Phase region boundary   6 at:   2.256E-01  1.185E+03
  ** BCC_A2
     QUASI
 Calculated..                      20  equilibria
 Terminating at axis limit.

 Phase region boundary   7 at:   0.000E+00  1.185E+03
  ** BCC_A2
     FCC_A1

 Phase region boundary   8 at:   0.000E+00  1.667E+03
     BCC_A2
  ** FCC_A1

 Phase region boundary   9 at:   6.305E-02  1.667E+03
  ** BCC_A2
     QUASI
 Calculated                      65  equilibria

 Phase region boundary  10 at:   2.243E-01  1.200E+03
  ** FCC_A1
     QUASI
 Calculated.                       3  equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   2.243E-01  1.200E+03
  ** FCC_A1
     QUASI
 Calculated.                     260  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex50\tcex
 50.POLY3
 CPU time for mapping                       8  seconds
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: set-title Fe-S fcc/liq and bcc/liq
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

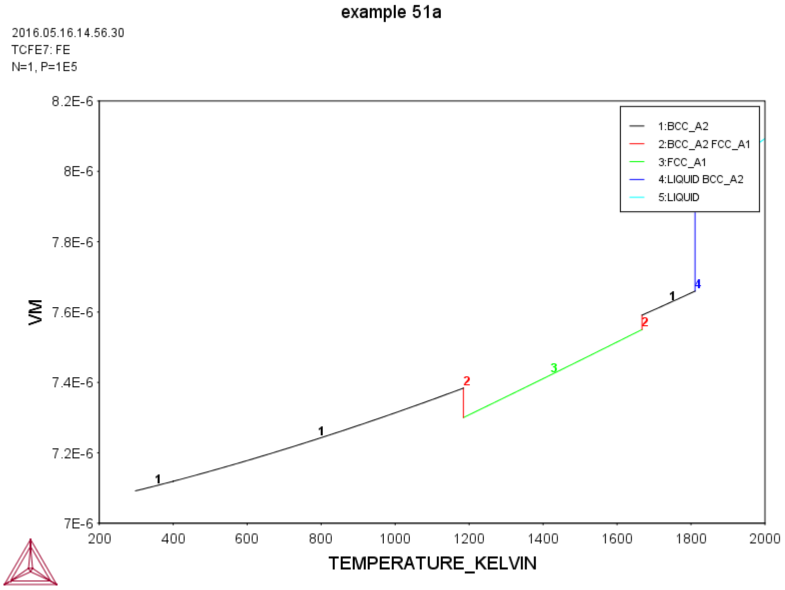


```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

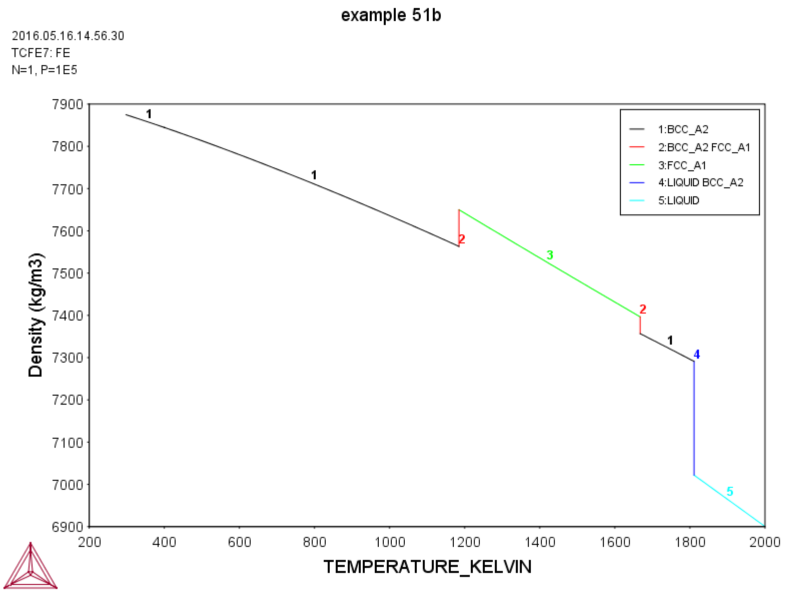
tcex51

```
SYS:About
 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 9533) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118
 License library version: 8.5.1.0017
 Linked: Mon May 16 09:31:44 2016


SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex51\tcex51.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of molar volume, thermal expansivity and density.
SYS: @@
SYS:
SYS: set-log ex51,,
SYS:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: sw tcfe7
   ... the command in full is SWITCH_DATABASE
 Current database: Steels/Fe-Alloys  v7.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE7:
TDB_TCFE7: @@ volume of a unary system
TDB_TCFE7: d-sys fe
   ... the command in full is DEFINE_SYSTEM
 FE  DEFINED
TDB_TCFE7: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  A1_KAPPA                KAPPA
 LAVES_PHASE_C14  REJECTED
TDB_TCFE7: rest-ph fcc_a1,bcc_a2,liquid
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  LIQUID:L
   RESTORED
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
 -OK-
TDB_TCFE7:
TDB_TCFE7: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=400, n=1, p=1e5
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated              3 grid points in             0 s
POLY_3: s-a-v 1 t 298 2000,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: save tcex51 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    400.000
...OK

 Phase Region from    400.000     for:
     BCC_A2
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
 Global check of adding phase at  1.18481E+03
 Calculated    81 equilibria

 Phase Region from    1184.81     for:
     BCC_A2
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    1184.81     for:
     FCC_A1
 Global test at  1.26000E+03 .... OK
 Global test at  1.36000E+03 .... OK
```

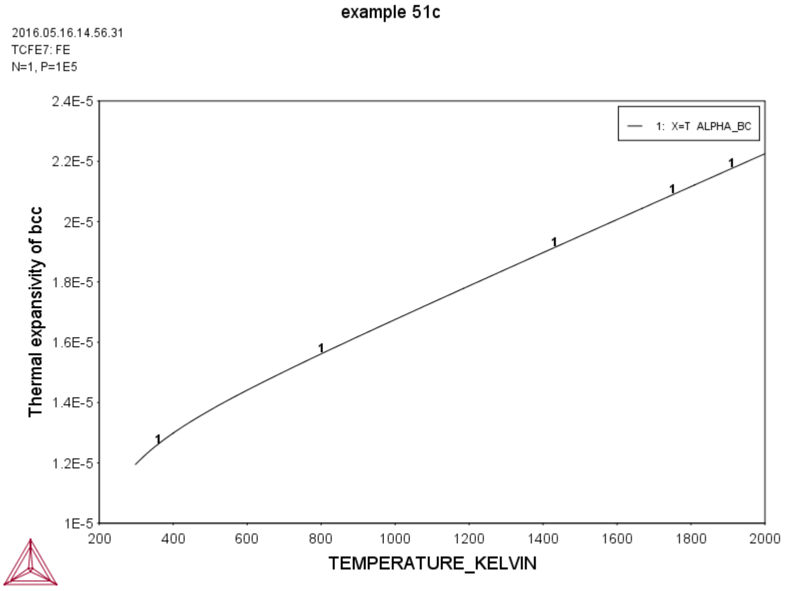
```
 Global test at  1.46000E+03 .... OK
 Global test at  1.56000E+03 .... OK
 Global test at  1.66000E+03 .... OK
 Global check of adding phase at  1.66747E+03
 Calculated    51 equilibria

 Phase Region from    1667.47     for:
     BCC_A2
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    1667.47     for:
     BCC_A2
 Global test at  1.74000E+03 .... OK
 Global check of adding phase at  1.81095E+03
 Calculated    18 equilibria

 Phase Region from    1810.95     for:
     LIQUID
     BCC_A2
 Calculated     2 equilibria

 Phase Region from    1810.95     for:
     LIQUID
 Global test at  1.89000E+03 .... OK
 Global test at  1.99000E+03 .... OK
 Terminating at    2000.00
 Calculated    22 equilibria

 Phase Region from    400.000     for:
     BCC_A2
 Global test at  3.20000E+02 .... OK
 Terminating at    298.000
 Calculated    14 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex51\tcex
 51.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51a
POST: s-l e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: @@ define and plot density
POST: ent fun density=b*1e-3/vm;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y density
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-axis-text y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Density (kg/m3)
POST: set-title example 51b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



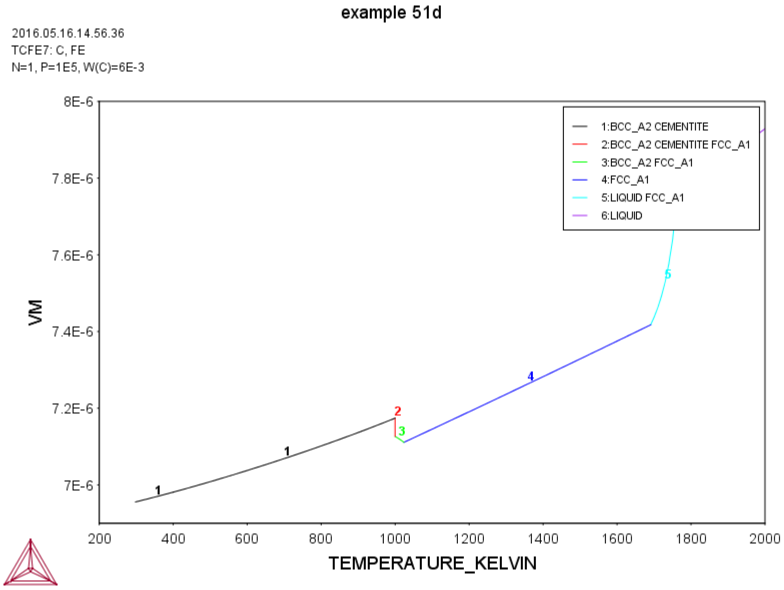
```
POST:
POST:Hit RETURN to continue
POST: @@ define and plot coefficient of linear
POST: @@  thermal expansion
POST: ent fun alpha_bcc_a2=vm(bcc_a2).t/vm(bcc_a2)/3;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y alpha_bcc_a2
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-axis-text y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Thermal expansivity of bcc
POST: set-title example 51c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST:Hit RETURN to continue
POST: back
POLY_3: @@ volume of Fe-C binary system
POLY_3: go da
   ... the command in full is GOTO_MODULE
TDB_TCFE7: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
TDB_TCFE7: de-sys fe c
   ... the command in full is DEFINE_SYSTEM
 FE                       C  DEFINED
TDB_TCFE7: rej-ph * all
   ... the command in full is REJECT
 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   DIAMOND_FCC_A4
 GRAPHITE                 CEMENTITE                M23C6
 M7C3                     M5C2                     KSI_CARBIDE
 A1_KAPPA                 KAPPA                    FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14  REJECTED
TDB_TCFE7: res-ph fcc_a1,bcc_a2,cementite,liquid
   ... the command in full is RESTORE
 FCC_A1                   BCC_A2                   CEMENTITE
 LIQUID:L  RESTORED
TDB_TCFE7: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
```

```
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 -OK-
TDB_TCFE7:
TDB_TCFE7: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=400, n=1, p=1e5
   ... the command in full is SET_CONDITION
POLY_3: s-c w(c)=.6e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           412 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 t 298 2000,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: save tcex51 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    400.000
...OK

 Phase Region from    400.000      for:
     BCC_A2
     CEMENTITE
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global check of adding phase at  9.99783E+02
 Calculated    62 equilibria

 Phase Region from    999.783      for:
     BCC_A2
     CEMENTITE
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    999.783      for:
     BCC_A2
     FCC_A1
 Global check of removing phase at  1.02363E+03
 Calculated     6 equilibria

 Phase Region from    1023.63      for:
     FCC_A1
 Global test at  1.10000E+03 .... OK
 Global test at  1.20000E+03 .... OK
 Global test at  1.30000E+03 .... OK
 Global test at  1.40000E+03 .... OK
 Global test at  1.50000E+03 .... OK
 Global test at  1.60000E+03 .... OK
 Global check of adding phase at  1.69090E+03
 Calculated    70 equilibria

 Phase Region from    1690.90      for:
     LIQUID
     FCC_A1
 Global check of removing phase at  1.76294E+03
 Calculated    10 equilibria

 Phase Region from    1762.94      for:
     LIQUID
 Global test at  1.84000E+03 .... OK
 Global test at  1.94000E+03 .... OK
 Terminating at    2000.00
 Calculated    27 equilibria

 Phase Region from    400.000      for:
     BCC_A2
     CEMENTITE
 Global test at  3.20000E+02 .... OK
 Terminating at    298.000
 Calculated    14 equilibria
 *** Buffer saved on file:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex51\tcex
 51.POLY3
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: s-d-a x t-k
```

```
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51d
POST: s-l e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex52

```
AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex52\tcex52.TCM"SYS: set-echo
SYS: @@
SYS: @@ Changing the excess models for interaction
SYS: @@ parameters in a solution phase
SYS: @@
SYS: @@ Example showing how to change the excess models for binary/ternary
SYS: @@ interactions in a solution phase, either through direct interactive
SYS: @@ amendments of phase descriptions within the GES module, or enforced
SYS: @@ by specific type-definitions given in a database file retrieved by
SYS: @@ the TDB module.
SYS: @@
SYS: @@  ------------------------------------------------------------------
SYS: @@   For Binary Excess Model:
SYS: @@           from the default R-K model   to Mixed-Excess-Model
SYS: @@                  (Note the phase has to be a substitutional phase)
SYS: @@  ------------------------------------------------------------------
SYS: @@   For Ternary Extrapolation Model:
SYS: @@           from the default R-K-M model to Toop_Kohler model
SYS: @@
SYS:
SYS: set-log TCEX52.LOG
Heading: Example showing how to enter a TOOP binary extrapolation model
SYS:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
TDB_TCFE8:
TDB_TCFE8: go gibbs
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES:
GES: ent-el  /- VA A B C
   ... the command in full is ENTER_ELEMENT
GES:
GES: am_el_d /-  ELECTRON_GAS           0.0000E+00  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d VA  VACUUM                 0.0000E+00  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d A   UNKNOWN                1.0000E+01  0.0000E+00  0.0000E+00 2
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d B   BETA_RHOMBO_B          1.0811E+01  1.2220E+00  5.9000E+00 2
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d C   GRAPHITE               1.2011E+01  1.0540E+00  5.7400E+00 2
   ... the command in full is AMEND_ELEMENT_DATA
GES:
GES: ent-phase LIQUID  L,  1   A,B,C ;  N N
   ... the command in full is ENTER_PHASE
GES:
GES: ent-param G(LIQUID,A;0) 298.15 0; 6000 N!
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A;0)-H298(UNKNOWN,A;0)
GES: ent-param G(LIQUID,B;0) 298.15 0; 6000 N!
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0)
GES: ent-param G(LIQUID,C;0) 298.15 0; 6000 N!
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,C;0)-H298(GRAPHITE,C;0)
GES:
GES: ent-param L(LIQUID,A,B;0)  298.15  10000;  6000 N
   ... the command in full is ENTER_PARAMETER
 L(LIQUID,A,B;0)
GES: ent-param L(LIQUID,A,B;1)  298.15 -10000;  6000 N
   ... the command in full is ENTER_PARAMETER
 L(LIQUID,A,B;1)
GES:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE: UNKNOWN

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00


 SPECIES                                    STOICHIOMETRY
   1 A                                      A
   2 B                                      B
   3 C                                      C
   4 VA                                     VA

 Sorry, no data output from this database


 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE
```

```
GES:Hit RETURN to continue
GES:
GES: @@
GES: @@ First Step: Amending the binary excess model:
GES: @@ *********** =====================================================
GES: @@ The default binary excess model is the Redlich-Kister Model for all
GES: @@  the three associated binary interaction pairs (A-B, A-C and B-C)
GES: @@  in the substitutional LIQUID solution phase (without sublattice)
GES: @@  that consists of three elements (A, B and C).
GES: @@
GES: @@ Before changing this default binary excess model for the ternary
GES: @@  LIQUID solution phase, one must have already entered the G
GES: @@  parameters (for standard Gibbs energies of all pure end-members)
GES: @@  and L parameters (for binary R-K excess interaction energies),
GES: @@  as shown here!
GES: @@
GES: @@ In this particular example, we want to change from the default R-K
GES: @@  binary excess model to the Mixed-Excess-Model (with three different
GES: @@  binary excess models, namely Legendre, Polynom and Redlich-Kister
GES: @@  models, applied to the A-B, A-C and B-C binaries, respectively),
GES: @@  as demonstrated below:
GES: @@
GES:
GES: @@... For the A-B interaction, the Legendre binary excess model should
GES: @@      be used (rather than the default Redlich-Kister Model), with
GES: @@      the first species (i.e. A) as the independent constituent
GES: @@      and the second species (i.e. B) as the dependent constituent,
GES: @@      while the L parameters for the A-B interaction shall remain
GES: @@      the same as those handled by the R-K model.
GES: @@
GES: amend-phase-description liquid
AMEND WHAT /COMPOSITION_SETS/: ?
 You can amend
 EXCESS_MODEL
 MAGNETIC_ORDERING
 DEBYE_HUCKEL
 STATUS_BITS
 NEW_CONSTITUENT
 RENAME_PHASE
 COMPOSITION_SETS
 GLASS_TRANSITION
 DISORDERED_PART
 MAJOR_CONSTITUENT
 ZRO2_TRANSITION
 REMOVE_ADDITIONS
 QUASICHEM_IONIC
 QUASICHEM_FACT00
 QUASICHEM_IRSID
 TERNARY_EXTRAPOLAT
 HKF_ELECTROSTATIC
 DEFAULT_STABLE
 SITE_RATIOS
 FRACTION_LIMITS
 NEVER_DISORDER_PAR
AMEND WHAT /COMPOSITION_SETS/: excess
MODEL NAME /REDLICH-KISTER_MUGGIANU/: ?
 REDLICH-KISTER_MUGGIANU
 REDLICH-KISTER_KOHLER
 FLORY-HUGGINS POLYMER MODEL
 MIXED-EXCESS-MODELS (R-K default)
 HKF
 PITZER
 CENTRAL_ATOM_MODEL

MODEL NAME /REDLICH-KISTER_MUGGIANU/: mixed
First (the independent) constituent: ?

 First (the independent) constituent

  Specify the first (the independent) constituent of a certain binary pair
  of constituents in the current substitutional solution phase, for which you
  wish to change the binary excess model from the default REDLICH-KISTER
  model to another model (LEGENDRE or POLYNOM). This sub-option will be
  repeatedly prompted (again and again), after having specified the desired
  binary Excess model type, for further changes of binary excess model for
  other specific binary pair in the current substitutional solution phase.

  By simply typing <RETURN> at such a repeated prompt (implying that there
  will be no more changes of binary excess model for all other possibly-
  remaining binary pairs that shall still use the default REDLICH-KISTER
  model), you can finish this MIXED-EXCESS-MODELS option.


First (the independent) constituent: A
Second (the dependent) constituent: B
Excess model type: /LEGENDRE/: ?
Legal choices are: LEGENDRE, POLYNOM or REDLICH-KISTER
Excess model type: /LEGENDRE/: legendre

 Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent: NONE
GES:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE:

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00


 SPECIES                                    STOICHIOMETRY
   1 A                                      A
   2 B                                      B
```

```
   3 C                                       C
   4 VA                                      VA

 Sorry, no data output from this database


 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE

GES:Hit RETURN to continue
GES:
GES: @@... For the A-C interaction, the Polynom binary excess model should
GES: @@      be used (rather than the default Redlich-Kister Model), with
GES: @@      the second species (i.e. C) as the independent constituent
GES: @@      and the first species (i.e. A) as the dependent constituent,
GES: @@      while the L parameters for the A-C interaction shall remain
GES: @@      the same as those handled by the R-K model.
GES: @@
GES: ent-param G(LIQUID,A,C;0)  298.15 10000;   6000 N
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A,C;0)
GES: ent-param G(LIQUID,A,C;1)  298.15  5000;   6000 N
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A,C;1)
GES:
GES: amend-phase-des LIQUID excess mixed C A polynom
   ... the command in full is AMEND_PHASE_DESCRIPTION

 Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE:

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00


 SPECIES                                     STOICHIOMETRY
   1 A                                       A
   2 B                                       B
   3 C                                       C
   4 VA                                      VA

 Sorry, no data output from this database


 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE

GES:Hit RETURN to continue
GES:
GES: @@... For the B-C interaction, the default Redlich-Kister binary
GES: @@      excess model shall still be used; so we do not need to amend
GES: @@      anything regarding that.
GES: @@
GES: ent-param G(LIQUID,B,C;0)  298.15 10000;   6000 N
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,B,C;0)
GES: ent-param G(LIQUID,B,C;1)  298.15 -2000;   6000 N
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,B,C;1)
GES:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE:

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00


 SPECIES                                     STOICHIOMETRY
   1 A                                       A
   2 B                                       B
   3 C                                       C
   4 VA                                      VA

 Sorry, no data output from this database


 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C
 No data listing for this database
```

```
 LIST_OF_REFERENCES
 NUMBER  SOURCE

GES:Hit RETURN to continue
GES:
GES: @@
GES: @@Second Step: Amending the ternary extrapolation model:
GES: @@************ =======================================================
GES: @@The default ternary excess model is the Redlich-Kister_Muggianu
GES: @@ Model (i.e., the MUGGIANU_RESTOR method for ternary extrapolation
GES: @@ based on binary parameters) for the associated ternary interaction
GES: @@ terms; when no ternary L parameter is entered for that, such a
GES: @@ default Redlich-Kister_Muggianu Model is thus to be used for
GES: @@ extrapolation from binary excess energies to ternary interactions
GES: @@ in the substitutional LIQUID solution phase (without sublattice)
GES: @@ that consists of three elements (A, B and C).
GES: @@
GES: @@However, in this particular example as illustrated in the following,
GES: @@ we shall change from this default R-K-M ternary excess model to
GES: @@ the TOOP-KOHLER method for the ternary extrapolation method, with
GES: @@ the species C as the Toop constituent, while the species A and B
GES: @@ as the Kohler constituents (entering A and B, or B and A, as the
GES: @@ basis constituent and first interacting constituent). This will
GES: @@ implicitly enforce that, during the ternary extrapolation, only
GES: @@ the A-B binary interaction parameters are utilized in accordance
GES: @@ with the Kohler ternary extrapolation formula for A-B-C ternary
GES: @@ interaction, while any other binary interaction parameters
GES: @@ involving the Toop species C (i.e., of A-C and B-C binaries) are
GES: @@ used in line with the Toop-Kohler ternary extrapolation formula
GES: @@ (for the A-C-B and B-C-A ternary interactions). This makes the
GES: @@ extrapolated ternary excess interaction terms different from
GES: @@ those handled either by the default MUGGIANU_RESTOR method
GES: @@ or by the alternative KOHLER-ALL method.
GES: @@
GES: @@Note that only when all the relevant binary excess energies in a
GES: @@ ternary system are treated by the default Redlich-Kister Model
GES: @@ (i.e., the Mixed-Excess-Model should have not been used), the
GES: @@ MUGGIANU_RESTOR method for ternary extrapolations is equivalent
GES: @@ to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method
GES: @@ to the Redlich-Kister_Kohler Model.
GES: @@
GES: amend_phase-des LIQUID
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: ?
 You can amend
 EXCESS_MODEL
 MAGNETIC_ORDERING
 DEBYE_HUCKEL
 STATUS_BITS
 NEW_CONSTITUENT
 RENAME_PHASE
 COMPOSITION_SETS
 GLASS_TRANSITION
 DISORDERED_PART
 MAJOR_CONSTITUENT
 ZRO2_TRANSITION
 REMOVE_ADDITIONS
 QUASICHEM_IONIC
 QUASICHEM_FACT00
 QUASICHEM_IRSID
 TERNARY_EXTRAPOLAT
 HKF_ELECTROSTATIC
 DEFAULT_STABLE
 SITE_RATIOS
 FRACTION_LIMITS
 NEVER_DISORDER_PAR
AMEND WHAT /COMPOSITION_SETS/: TERN-EXT
Extrapolation method: /TOOP-KOHLER/: ?
 Default method is Muggianu, you can use
 TOOP-KOHLER
 KOHLER-ALL
 MUGGIANU_RESTOR
Extrapolation method: /TOOP-KOHLER/: TOOP-KOHLER
Constituent in sublattice 1: A
First interaction constituent: B
Toop constituent: C
GES:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2016- 5-16
 FROM DATABASE:

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00


 SPECIES                                    STOICHIOMETRY
   1 A                                      A
   2 B                                      B
   3 C                                      C
   4 VA                                     VA

 Sorry, no data output from this database


 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE

GES:Hit RETURN to continue
```

```
GES:
GES: @@ Third Step: Performing an equilibrium calculation
GES: @@               using the entered and amended descriptions.
GES: @@ *********** ========================================================
GES: @@
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e , X
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database:

 Conditions:
 T=1500, P=1E5, N=1, X(B)=0.2, X(C)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1500.00 K (  1226.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.07655E+01
 Total Gibbs energy -1.08432E+04,  Enthalpy  1.99843E+03,  Volume  0.00000E+00

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 A                        5.0000E-01  5.0000E-01 4.7833E-01 -9.1973E+03 SER
 B                        2.0000E-01  2.0000E-01 1.9875E-01 -2.0151E+04 SER
 C                        3.0000E-01  3.0000E-01 5.5332E-01 -7.3811E+03 SER

 LIQUID                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0765E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.00000E-01  C  3.00000E-01  B  2.00000E-01
POLY_3: sh qf(*)
   ... the command in full is SHOW_VALUE
 QF(LIQUID)=0.52168269
POLY_3: sh gm(*) dgm(*)
   ... the command in full is SHOW_VALUE
 GM(LIQUID)=-10843.162
 DGM(LIQUID)=0
POLY_3:
POLY_3: save TCEX52a.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: @@ Fourth Step: Reading the same data from a small database and
POLY_3: @@              Performing the same equilibrium calculation.
POLY_3: @@ ************ ========================================================
POLY_3: @@
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE8: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 L12_FCC                  B2_BCC                   B2_VACANCY
 HIGH_SIGMA               DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
TDB_TCFE8:
TDB_TCFE8: sw user TCEX52-TOOP.TDB
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                       /-   DEFINED
TDB_USER: d-sys /all
   ... the command in full is DEFINE_SYSTEM
 A                        B                        C
   DEFINED
TDB_USER: l-sys const
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :A B C:
TDB_USER: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Reference 2'
  'Reference 1'
 AFTER ...
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 -OK-
TDB_USER:
TDB_USER:Hit RETURN to continue
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3:
POLY_3: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1977 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e , X
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1500, P=1E5, N=1, X(B)=0.2, X(C)=0.3
 DEGREES OF FREEDOM 0
```

```
 Temperature   1500.00 K (  1226.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.07655E+01
 Total Gibbs energy -1.08432E+04,  Enthalpy  1.99843E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       5.0000E-01  5.0000E-01 4.7833E-01 -9.1973E+03 SER
 B                       2.0000E-01  2.0000E-01 1.9875E-01 -2.0151E+04 SER
 C                       3.0000E-01  3.0000E-01 5.5332E-01 -7.3811E+03 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0765E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.00000E-01  C  3.00000E-01  B  2.00000E-01
POLY_3: sh qf(*)
   ... the command in full is SHOW_VALUE
 QF(LIQUID)=0.52168269
POLY_3: sh gm(*) dgm(*)
   ... the command in full is SHOW_VALUE
 GM(LIQUID)=-10843.162
 DGM(LIQUID)=0
POLY_3:
POLY_3: save TCEX52b.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: @@
POLY_3: @@ As you have noticed above, the calculated equilibrium (using the
POLY_3: @@   small database) is exactly the same as the first calculation
POLY_3: @@   (with data amended in the GES module step-by-step, for the
POLY_3: @@   binary/ternary excess models).
POLY_3: @@
POLY_3:
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3:
```

tcex53

```
AboutSYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex53\tcex53.TCM"SYS:SYS:SYS:
SYS:
SYS:SYS: set-echo
SYS:
SYS: set-log TCEX53.LOG
Heading: Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine
SYS:
SYS: @@
SYS: @@ TCEX53: Thermo-Calc 4.0 (Console Mode) Standard Example No 53
SYS: @@ ******* ============================================================
SYS: @@   Copyright: Thermo-Calc Software AB, Stockholm, Sweden
SYS: @@   Developer: Dr. Pingfang Shi, Thermo-Calc Software AB
SYS: @@   Date:      2014-05-26 (revision)
SYS: @@
SYS: @@ Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine
SYS: @@ *******************************************************************
SYS: @@    * Using PAQ2 or PAQS2 database;
SYS: @@    * For the Fe-X-H2O-NaCl heterogeneous interaction systems
SYS: @@                (X = Cr-Ni-Co)
SYS: @@ ===================================================================
SYS: @@ Note: The PAQ2 (TCS Public Aqueous Solution (SIT) Database, v2.4;
SYS: @@         using the SIT aqueous solution model) or PAQS2 (TCS Public
SYS: @@         Aqueous Solution Database, v2.4; using the Complete Revised
SYS: @@         HKF aqueous solution model) contains an AQUEOUS solution
SYS: @@         phase and REF_ELECTRODE phase (as a reference for electron
SYS: @@         in aqueous electrolyte systems), as well as some data for
SYS: @@         various solid phases (solution or stoichiometric) and
SYS: @@         gaseous mixture phase. Therefore, it can be used, via the
SYS: @@         Single-Database Option in the POURBAIX module or through
SYS: @@         the normal TDB-GES-PLOY-POST routine, for calculations of
SYS: @@         the so-called Pourbaix diagrams (i.e., pH-Eh plots) and
SYS: @@         other types of diagrams in aqueous-bearing multicomponent
SYS: @@         heterogeneous interaction systems.
SYS: @@ -------------------------------------------------------------------
SYS: @@ Also Note: The initial bulk composition of Fe-based alloy in this
SYS: @@              demonstrating calculation is just preliminarily assigned,
SYS: @@              in which the BCC_A2 and/or FCC_A1 solution phase(s) are
SYS: @@              considered as of primarily interest.
SYS: @@            For practical calculations, one shall have more precise
SYS: @@              inputs for the initial bulk compositions of alloys.
SYS: @@ -------------------------------------------------------------------
SYS: @@
SYS:
SYS: @@ ===================================================================
SYS: @@ Step 1: Single-Point Calculations for H2O-NaCl system
SYS: @@ *******************************************************************
SYS: @@   To demonstrate how to define the molality of NaCl
SYS: @@       in an aqueous-bearing heterogeneous interaction system
SYS: @@
SYS:
SYS: @@... Retrieving data from the PAQ2 or PAQS2 database:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Current database: Steels/Fe-Alloys  v8.0

 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
TDB_TCFE8: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 L12_FCC                 B2_BCC                  B2_VACANCY
 HIGH_SIGMA              DICTRA_FCC_A1  REJECTED
 REINITIATING GES5 .....
TDB_TCFE8: @@ ------ switch on PAQ2 or PAQS2
TDB_TCFE8: sw PAQ2
   ... the command in full is SWITCH_DATABASE
 Current database: Public Aqueous Soln (SIT) TDB v2.4

 H                       O                       ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                DIAMOND_A4              FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                CUB_A13                 CHI_A12
 FE4N                    FECN_CHI  REJECTED
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 PI  REJECTED
 FE3C                    NI3C                    CR3C2
 CR7C3                   CR23C6  REJECTED
 COCO3                   FECO3                   NAHCO3
 NA2CO3                  NA2CO3_S2               NICO3
 CRC6O6  REJECTED
 CO3N                    CRN                     CR2N
 FE2N                    NI3N  REJECTED
 NANO2                   NANO2_S2                NANO3
   REJECTED
 COCL2                   CRCL2                   CRCL3
 FECL2                   FECL3                   NICL2
   REJECTED
 FECLO                   NACLO4                  NACLO4_S2
   REJECTED
TDB_PAQ2: data
   ... the command in full is DATABASE_INFORMATION
 Current database: Public Aqueous Soln (SIT) TDB v2.4

                                     PAQ2
              Thermo-Calc PUBLIC AQUEOUS DATABASE FOR POURBAIX MODULE
         (based on and replacing AQ in TCC/TCW & PAQ in TCC-Demo/TCW-Demo)
        ********************************************************************
                           (Version 2.4, Feb. 2008)

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   This public aqueous solution database contains aqueous solution species,
   and gaseous mixture species and solid/liquid (pure and solution) phases
   in an 11-element system (Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl). As a demo version
   of the complete TCAQ2 Aqueous Solution Database, it is specially designed
```

```
   for uses with the apecial POURBAIX module which allows easy and automatic
   calculations of the sp-called Pourbaix diagrams (i.e., Eh-pH plots) and
   many types of property diagrams. It can also be used in normal TCC/TCW
   calculations for aqueous involved hetergeneous interaction systems.

   The TCAQ2 Aqueous Solution Database covers 83 elements (compatible with
   the SGTE PURE/SSUB/SSOL and other databases), and can be used together
   with the SIT (Specific Interaction Theory) Model for complex aqueous
   solution that has already implemented in Thermo-Calc.

   PAQ has been developed since 1996, and gradually modified and expanded
   later on. PAQ2.4 combines 4 files from its previous version PAQ2 [i.e.,
   PAQ2setup.TDB for defining elements, species and phases; PAQ2param.TDB
   for assigning various functions and parameters for standard properties
   of various phases; PAQ2inter.TDB for assigning binary or higher-order
   interaction parameters for non-ideal properties of aqueous solution
   phase; and PAQ2funct.TDB for entering extra functions referred in
   PAQ2param.TDB].

   The AQUEOUS solution phase can be treated by the SIT Model, using the
   TCAQ2 (or PAQ2) database that can be applied to low PTX conditions (up
   to 100 bar, 350 C and 3 molality). However, if investigated hetergeneous
   interaction processes occur at high PTX (up to 5 kbar, 1000 C and 10
   molality), the other aqueous solution database, called AQS2, which
   implies the complete Revised HKF (Helgeson-Kirkham-Flowers) Model, is
   required.

   Data for pure elements are taken from the SGTE unary database (PURE) with
   explicit magnetic and pressure dependencies. The reference state is
   298.15 K and 1 bar. All data follow the new temperature scale ITPS 90.

   For calculations of the so-called Pourbaix-diagrams (pH-Eh) and related
   property diagrams within either the POURBAIX-module or through normal
   TDB-GES-POLY-POST routines, following types of phases must be defined
   in the heterogeneous interaction systems:
     AQUEOUS:        from PAQ2 (or PAQS2) or TCAQ2 (or AQS2);
     REF_ELECTRODE:  from PAQ2 (or PAQS2) or TCAQ2 (or AQS2);
     GAS:            from PAQ2 (or PAQS2) or SSUB4 (or TCMP2);
     Various Solids: from PAQ2 (or PAQS2) or SSOL4 (or TCFE6, TCMP2, etc.).
   There are many solid phases (stoichiometric or solution) and a metallic
   liquid mixture phase which are included in the public PAQ2 and PAQS2
   databases. By default, however, many such phases have been rejected
   automatically. Of course, if one wishes to consider any of such phases
   (such as Cementite or M23C6) into a defined interaction system, they
   can be appropriately restored in the POURBAIX or TDB modules.

   Either TCAQ2 or AQS2 databases can be used by the advanced, easy-to-use
   POURBAIX Module via its multiple-database option, or be utilized along
   with ordinary Thermo-Calc routines. For a gaseous mixture phase, one
   could append from the SSUB (SGTE PURE SUBSTANCES DATABASE, which treats
   the gas phase as an ideal mixture at all temperatures, pressures and
   compositions), or from some non-ideal gaseous/fluid mixture models
   implemented in the Thermo-Calc GES system (such as the SUPERFLUID model,
   i.e., the non-ideal EOS and non-ideal mixing for the C-H-O-S-N-Ar fluids;
   Shi and Saxena, 1992). For other condensed materials except for aqueous
   solution species, one could append data (of stoichiometric and solution
   solid phases) from any compatible Thermo-Calc database(s) [e.g., PURE,
   SSUB, SSOL, TCFE, TCNI, TCNF, CCC1, TTNi, TTTi, TTAl, TTMg, TTZr, NSLD,
   SEMC, TCMP, TCES, SALT, ION, SLAG, NOX, NUOX, SNUX, NUMT, GCE, and other
   substances/solutions databases), depending upon application systems and
   investigated aqueous-bearing heterogeneous interaction processes.

   In a normal POLY calculation (single points, stepping, and/or mapping),
     one should always remember as the first step to appropriately redefine
     the components as follows:
       DEF-COMP H2O H+1 Ze Fe Ni NaCl Cl-1 S <& other components> ;
    Then, one can appropriately define the equilibrium conditions, e.g.,
       SET-COND P=1e5 T=300 B=1000 N(H+1)=0 N(Ze)=0 N(Fe)=1e-6 N(NaCl)=3...;
      and set the necessary reference states for some components, e.g.,
       SET-REFERENCE-STATE H2O AQUEOUS * 1E5 ;
       SET-REFERENCE-STATE ZE REF_ELEC * 1E5 ;
       SET-REFERENCE-STATE NaCl HALITE * 1E5 ;
       SET-REFERENCE-STATE Fe BCC * 1E5 ;
    The pH and Eh are thus defined by entering the following functions:
       ENT-SYM FUNC pH=-log10(ACR(H+1)) ;
       ENT-SYM FUNC Eh=MUR(ZE)/RNF ;
      However, if the reference state for H+1 component has been defined by
       SET-REFERENCE-STATE H+1 AQUEOUS * 1E5 ;
      then the pH quantity should be alternatively entered as:
       ENT-SYM FUNC pH=-log10(ACR(H+1,AQUEOUS)) ;

    For defining activity and activity coefficients of the solvent, use:
       ENT-SYM FUNC ACRH2O=ACR(H2O,AQUEOUS) ;
       ENT-SYM FUNC RCH2O=ACR(H2O,AQUEOUS) ;
      while for defining activity, activity coefficients and molality of
      a specific solute species "i", use:
       ENT-SYM FUNC AIi=ACR(i,AQUEOUS)*AH2O ;
       ENT-SYM FUNC RCi=ACR(i,AQUEOUS)*YH2O/Y(AQUEOUS,i) ;
       ENT-SYM FUNC MLi=Y(AQUEOUS,i)*AH2O/YH2O ;
      where RNF=96485.309, AH2O=55.508435 and YH2O=Y(AQUEOUS,H2O) as
      predefined functions, and i=Fe+2 (for instance) as species name.

   Important Note: The REF_ELECTRODE phase is the reference electrode which
   should always be included in a defined system involving aqueous solution
   for the purpose of calculating electron potentail [MUR(ZE)], while this
   phase should always be SUSPENDED in all the POLY calculations.

   For further information, please contact Dr. Pingfang Shi at TCSAB.

   Release History: Version 1.0 initial release (as AQ),             1997
                    Version 1.1 with minor improvements (as AQ),     1998
                    Version 1.2 with minor improvements (as AQ),     2000
                    Version 2.0 with major improvements (as PAQ2.0), 2002
                    Version 2.1 with minor improvements (as PAQ2.1), 2003
                    Version 2.2 with minor improvements (as PAQ2.2), 2006
                    Version 2.3 with minor improvements (as PAQ2.3), 2007
                    Version 2.4 with major improvements (as PAQ2.4), 2008

   Edited by: Dr. Pingfang Shi (Thermo-Calc Software, 1997-2008).
   ========================================================================

TDB_PAQ2: d-sys H O Na Cl
   ... the command in full is DEFINE_SYSTEM
 NA                      CL  DEFINED
TDB_PAQ2: l-sys const
   ... the command in full is LIST_SYSTEM
```

```
 AQUEOUS:A   :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CL2 CL-1 CLO2 CLO-1 CLO2-1
  CLO3-1 CLO4-1 HCLO HCLO2 NA+1:
  > Aqueous Solution: using the SIT Model (from TCAQ2 database)
 REF_ELECTRODE :ZE:
  > Reference Electrode for ZE potentail; always SUSPENDED in POLY.
 GAS:G       :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1NA1 CL2NA2 CL3NA3 H
  H1NA1 H1NA1O1 H1O1 H1O2 H2 H2NA2O2 H2O1 H2O2 NA NA1O1 NA2 NA2O1 NA2O2 O O2
  O3:
  > Gaseous Mixture, using the ideal gas model
 FCC_A1      :NA O:VA:
  > This is also the MX (X=C,N) solution phase.
 BCC_A2      :NA O:VA:
  > This is also the MX3 (X=C,N) solution phase.
 HCP_A3      :NA:VA:
  > This is also the M2X (X=C,N) solution phase.
 HALITE      :NA1CL1:
 NAO2        :NA1O2:
 NA2O        :NA2O1:
 NA2O_S2     :NA2O1:
 NA2O_S3     :NA2O1:
 NA2O2       :NA2O2:
 NA2O2_S2    :NA2O2:
 NAOH        :H1NA1O1:
 NAOH_S2     :H1NA1O1:
TDB_PAQ2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
      -Cl system.'
  'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
      -Cr-Na-Ni-C-H-O-N-S-Cl system.'
  'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
      -Na-Ni-C-H-O-N-S-Cl system.'
  'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
      only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
      from TCAQ2 which covers totally 83 elements and contains many more
      aqueous solution species.'
 -OK-
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: @@... Defining system-components and their proper reference states:
TDB_PAQ2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: d-com H2O H+1 ZE Na Cl
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-r-s H2O AQUEOUS * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s ZE  REF_ELE * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H2O                     ENTERED   AQUEOUS        *              100000
 H+1                     ENTERED   SER
 ZE                      ENTERED   REF_ELECTRODE  *              100000
 NA                      ENTERED   SER
 CL                      ENTERED   SER
POLY_3:
POLY_3: @@... Defining the equilibrium conditions:
POLY_3: @@    -------------------------------------------------------------
POLY_3: @@     Defining P-T and bulk composition in the interaction system
POLY_3: @@     for the calculations of initial equilibria:
POLY_3: @@
POLY_3: s-c P=1e5 T=298.15 b(H2O)=1000
   ... the command in full is SET_CONDITION
POLY_3: s-in-am b(Na1Cl1)=5
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-c n(H+1)=0 n(ZE)=0
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
    N(ZE)=0
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: @@... Calculating an equilibrium with only AQUEOUS presented:
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 AQUEOUS                 ENTERED      0.000000E+00    1.785600E+03
 SUSPENDED PHASES:
 REF_ELECTRODE NAOH_S2 NAOH NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O HCP_A3
 HALITE FCC_A1 BCC_A2 GAS
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated            17 grid points in               0 s
Found the set of lowest grid points in                0 s
 Creating a new composition set AQUEOUS#2
 Creating a new composition set AQUEOUS#3
 Calculated POLY solution       0 s, total time     0  s
```

```
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
    N(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.56795E+01,  Mass in grams  1.00500E+03
 Total Gibbs energy -1.70630E+07,  Enthalpy -1.59010E+07,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                     5.5508E+01  9.9693E-01 9.9654E-01 -8.5871E+00 AQUEOUS
 H+1                    -9.7239E-08 -1.7464E-09 1.0405E-07 -3.9858E+04 SER
 ZE                      8.6043E-08  1.5453E-09 3.4476E+12  7.1565E+04 REF_ELEC
 NA                      8.5554E-02  1.5365E-03 4.5046E-63 -3.5588E+05 SER
 CL                      8.5554E-02  1.5365E-03 4.1623E-18 -9.9210E+04 SER

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00  Mole fractions:
 H2O  9.96927E-01  NA   1.53654E-03  H+1 -1.74641E-09
 CL   1.53654E-03  ZE   1.54532E-09
 Constitution:           SiteFraction    Molality      Activity    log10Act
 H2O                      9.96927E-01   5.55084E+01   9.96605E-01    -0.0015
 CL-1                     1.53654E-03   8.55538E-02   6.73425E-02    -1.1717
 NA+1                     1.53654E-03   8.55538E-02   6.73424E-02    -1.1717
 H+1                      2.37132E-09   1.32034E-07   1.04050E-07    -6.9828
 OH-1                     2.19965E-09   1.22476E-07   9.63757E-08    -7.0160
 O2                       4.70270E-10   2.61844E-08   2.61828E-08    -7.5820
 O3                       1.00000E-12   0.00000E+00   2.70935E-38   -37.5671
 HCLO                     1.00000E-12   0.00000E+00   3.25360E-20   -19.4876
 H2O2                     1.00000E-12   0.00000E+00   3.68420E-21   -20.4337
 HCLO2                    1.00000E-12   0.00000E+00   1.28717E-37   -36.8904
 H2                       1.00000E-12   0.00000E+00   5.39110E-43   -42.2683
 HO2-1                    1.00000E-12   0.00000E+00   7.49315E-26   -25.1253
 CLO4-1                   1.00000E-12   0.00000E+00   8.09139E-33   -32.0920
 CLO3-1                   1.00000E-12   0.00000E+00   1.41605E-30   -29.8489
 CLO2-1                   1.00000E-12   0.00000E+00   1.29472E-32   -31.8878
 CLO2                     1.00000E-12   0.00000E+00   4.84011E-38   -37.3151
 CLO-1                    1.00000E-12   0.00000E+00   6.77886E-21   -20.1688
 CL2                      1.00000E-12   0.00000E+00   4.80004E-25   -24.3188
 Solution Properties:   pH =    6.9828    Eh =    0.7417 V     I =    0.0856
                        pe =   12.5375    Ah =   71.5647 kJ   m* =    0.1711
                        Aw =    0.9966    Os =    1.1033     pKw =  13.9973
                        At1= 1.0000E-12  At2= 1.2248E-07 (equiv_mol/kg_H2O)
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 AQUEOUS                 ENTERED      0.000000E+00    5.567954E+01
 SUSPENDED PHASES:
 REF_ELECTRODE NAOH_S2 NAOH NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O HCP_A3
 HALITE FCC_A1 BCC_A2 AQUEOUS#3 AQUEOUS#2 GAS
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.
 N=55.679543
 N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042549E-8,
    N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: @@... Calculating an equilibrium with all phases presented:
POLY_3: @@                                       (except for REF_ELE)
POLY_3: c-st p *=ent 0
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY_3: @@ ...... Always setting the REF_ELECTRODE phase as SUSPENDED:
POLY_3: c-st p REF_ELE=sus
   ... the command in full is CHANGE_STATUS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 NAOH_S2                 ENTERED      0.000000E+00    0.000000E+00
 NAOH                    ENTERED      0.000000E+00    0.000000E+00
 NAO2                    ENTERED      0.000000E+00    0.000000E+00
 NA2O_S3                 ENTERED      0.000000E+00    0.000000E+00
 NA2O_S2                 ENTERED      0.000000E+00    0.000000E+00
 NA2O2_S2                ENTERED      0.000000E+00    0.000000E+00
 NA2O2                   ENTERED      0.000000E+00    0.000000E+00
 NA2O                    ENTERED      0.000000E+00    0.000000E+00
 HCP_A3                  ENTERED      0.000000E+00    0.000000E+00
 HALITE                  ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                  ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                  ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS#3               ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS#2               ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS                 ENTERED      0.000000E+00    5.580000E+01
 GAS                     ENTERED      0.000000E+00    0.000000E+00
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           679 grid points in               0 s
Found the set of lowest grid points in                0 s
 Calculated POLY solution       1 s, total time      1  s
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
    N(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.56795E+01,  Mass in grams  1.00500E+03
 Total Gibbs energy -1.70630E+07,  Enthalpy -1.59010E+07,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                     5.5508E+01  9.9693E-01 9.9654E-01 -8.5871E+00 AQUEOUS
```

```
 H+1                    -9.7239E-08 -1.7464E-09 1.0405E-07 -3.9858E+04 SER
 ZE                      8.6043E-08  1.5453E-09 3.4476E+12  7.1565E+04 REF_ELEC
 NA                      8.5554E-02  1.5365E-03 4.5046E-63 -3.5588E+05 SER
 CL                      8.5554E-02  1.5365E-03 4.1623E-18 -9.9210E+04 SER

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00  Mole fractions:
 H2O  9.96927E-01  NA   1.53654E-03  H+1 -1.74641E-09
 CL   1.53654E-03  ZE   1.54532E-09
 Constitution:           SiteFraction    Molality      Activity    log10Act
 H2O                      9.96927E-01   5.55084E+01   9.96605E-01    -0.0015
 CL-1                     1.53654E-03   8.55538E-02   6.73425E-02    -1.1717
 NA+1                     1.53654E-03   8.55538E-02   6.73424E-02    -1.1717
 H+1                      2.37132E-09   1.32034E-07   1.04050E-07    -6.9828
 OH-1                     2.19965E-09   1.22476E-07   9.63757E-08    -7.0160
 O2                       4.70270E-10   2.61844E-08   2.61828E-08    -7.5820
 O3                       1.00000E-12   0.00000E+00   2.70935E-38   -37.5671
 HCLO                     1.00000E-12   0.00000E+00   3.25360E-20   -19.4876
 H2O2                     1.00000E-12   0.00000E+00   3.68420E-21   -20.4337
 HCLO2                    1.00000E-12   0.00000E+00   1.28717E-37   -36.8904
 H2                       1.00000E-12   0.00000E+00   5.39110E-43   -42.2683
 HO2-1                    1.00000E-12   0.00000E+00   7.49315E-26   -25.1253
 CLO4-1                   1.00000E-12   0.00000E+00   8.09139E-33   -32.0920
 CLO3-1                   1.00000E-12   0.00000E+00   1.41605E-30   -29.8489
 CLO2-1                   1.00000E-12   0.00000E+00   1.29472E-32   -31.8878
 CLO2                     1.00000E-12   0.00000E+00   4.84011E-38   -37.3151
 CLO-1                    1.00000E-12   0.00000E+00   6.77886E-21   -20.1688
 CL2                      1.00000E-12   0.00000E+00   4.80004E-25   -24.3188
 Solution Properties:   pH =   6.9828    Eh =    0.7417 V     I =   0.0856
                        pe =  12.5375    Ah =   71.5647 kJ   m* =   0.1711
                        Aw =   0.9966    Os =    1.1033     pKw =  13.9973
                        At1= 1.0000E-12  At2= 1.2248E-07 (equiv_mol/kg_H2O)
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 AQUEOUS#3               ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS#2               ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS                 ENTERED      0.000000E+00    5.567954E+01
 GAS                     ENTERED     -3.453482E+00    0.000000E+00
 HALITE                  ENTERED     -4.519288E+00    0.000000E+00
 NAOH                    ENTERED     -1.737487E+01    0.000000E+00
 BCC_A2                  ENTERED     -1.752962E+01    0.000000E+00
 FCC_A1                  ENTERED     -1.752962E+01    0.000000E+00
 NAOH_S2                 ENTERED     -1.793977E+01    0.000000E+00
 NAO2                    ENTERED     -1.999496E+01    0.000000E+00
 NA2O2                   ENTERED     -2.605088E+01    0.000000E+00
 NA2O2_S2                ENTERED     -2.640940E+01    0.000000E+00
 NA2O                    ENTERED     -4.241247E+01    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -4.257992E+01
 NA2O_S2 NA2O_S3 HCP_A3
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.
 N=55.679543
 N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042557E-8,
    N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY_3: @@
POLY_3: @@ As shown here, 0.5wt% of NaCl (in 1 kg of H2O) is equivalent to
POLY_3: @@   0.085554 molality of NaCl.
POLY_3: @@
POLY_3:
POLY_3: @@... Saving the workspace for the H2O-NaCl system:
POLY_3: save TCEX53_a.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: @@ ====================================================================
POLY_3: @@ Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co) system
POLY_3: @@ ********************************************************************
POLY_3: @@   To demonstrate how to define the initial amount of alloy
POLY_3: @@       in an aqueous-bearing heterogeneous interaction system:
POLY_3: @@   -----------------------------------------------------------------
POLY_3: @@   Note: We are interested in only the BCC_A2 and FCC_A1 phases in
POLY_3: @@           the Fe-based alloy, in the current testing calculation.
POLY_3: @@         One may consider other possible phases (which exist in the
POLY_3: @@           applied steel material) if necessary.
POLY_3: @@
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_PAQ2: rej sys
   ... the command in full is REJECT
 H                       O                       ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                DIAMOND_A4              FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                CUB_A13                 CHI_A12
 FE4N                    FECN_CHI  REJECTED
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 PI  REJECTED
 FE3C                    NI3C                    CR3C2
 CR7C3                   CR23C6  REJECTED
 COCO3                   FECO3                   NAHCO3
 NA2CO3                  NA2CO3_S2               NICO3
 CRC6O6  REJECTED
 CO3N                    CRN                     CR2N
 FE2N                    NI3N  REJECTED
 NANO2                   NANO2_S2                NANO3
   REJECTED
 COCL2                   CRCL2                   CRCL3
 FECL2                   FECL3                   NICL2
   REJECTED
 FECLO                   NACLO4                  NACLO4_S2
   REJECTED
 REINITIATING GES5 .....
TDB_PAQ2:    sw PAQ2
   ... the command in full is SWITCH_DATABASE
TDB_PAQ2: rej ele H O ZE
   ... the command in full is REJECT
 H                       O                       ZE
```

```
   REJECTED
TDB_PAQ2: d-sys Fe Cr Ni Co
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      NI
 CO  DEFINED
TDB_PAQ2: l-sys const
   ... the command in full is LIST_SYSTEM
 GAS:G       :CO CR CR2 FE NI:
  > Gaseous Mixture, using the ideal gas model
 FCC_A1      :CO CR FE NI:VA:
  > This is also the MX (X=C,N) solution phase.
 BCC_A2      :CO CR FE NI:VA:
  > This is also the MX3 (X=C,N) solution phase.
 HCP_A3      :CO CR FE NI:VA:
  > This is also the M2X (X=C,N) solution phase.
 SIGMA       :CO FE NI:CR:CO CR FE NI:
TDB_PAQ2: rej-ph *
   ... the command in full is REJECT
 GAS:G                   FCC_A1                  BCC_A2
 HCP_A3                  SIGMA  REJECTED
TDB_PAQ2: rest-ph FCC_A1 BCC_A2
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2  RESTORED
TDB_PAQ2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
      -Cr-Na-Ni-C-H-O-N-S-Cl system.'
 -OK-
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3:
POLY_3: @@... One may turn on the Global Minimization in the calculations:
POLY_3:    Adv-Opt EQ_CALC Y Y !
   ... the command in full is ADVANCED_OPTIONS
 Settings for the minimization of an equilibra:
POLY_3:    Adv-Opt GLOBAL  Y 20000 !
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY_3:
POLY_3: s-c P=1e5 T=298.15
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@... The following conditions [system-size B and initial bulk
POLY_3: @@      composition w(i) of Fe-alloy] corresponds to the total
POLY_3: @@      initial amount of Fe-based alloy in the interaction,
POLY_3: @@      i.e., 1 gram of steel (Fe-10Cr-5Ni-1Co wt%).
POLY_3: s-c B=1  w(Cr)=.10 w(Ni)=.05 w(Co)=.01
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         39296 grid points in             0 s
Found the set of lowest grid points in              0 s
 Creating a new composition set BCC_A2#2
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.79859E-02,  Mass in grams  1.00000E+00
 Total Gibbs energy -1.58616E+02,  Enthalpy -1.09889E+01,  Volume  1.20553E-07

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 CO                      1.6968E-04  9.4342E-03 4.4157E-08 -4.1983E+04 SER
 CR                      1.9232E-03  1.0693E-01 5.8926E-02 -7.0192E+03 SER
 FE                      1.5041E-02  8.3627E-01 3.7073E-02 -8.1679E+03 SER
 NI                      8.5193E-04  4.7367E-02 7.7089E-04 -1.7769E+04 SER

 BCC_A2#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.4641E-02, Mass 8.1821E-01, Volume fraction 8.5170E-01  Mole fractions:
 FE  9.87131E-01  CO  1.15888E-02  NI  8.17873E-04  CR  4.61992E-04

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.9166E-03, Mass 9.9654E-02, Volume fraction 1.1495E-01  Mole fractions:
 CR  9.99946E-01  FE  5.39522E-05  CO  9.25541E-12  NI  8.81026E-12

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.4280E-03, Mass 8.2138E-02, Volume fraction 3.3346E-02  Mole fractions:
 NI  5.88202E-01  FE  4.11792E-01  CO  5.30943E-06  CR  6.98908E-09
POLY_3: l-st cp
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 CO                      ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 NI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
```

```
 FCC_A1                   ENTERED      0.000000E+00    1.428010E-03
 BCC_A2#2                 ENTERED      0.000000E+00    1.464136E-02
 BCC_A2                   ENTERED      0.000000E+00    1.916564E-03
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1.
 N=1.7985937E-2
 N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: s-c T=1073.15
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         39296 grid points in             1 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0

 Temperature   1073.15 K (   800.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.79859E-02,  Mass in grams  1.00000E+00
 Total Gibbs energy -9.18150E+02,  Enthalpy  5.59649E+02,  Volume  1.23044E-07

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 CO                       1.6968E-04  9.4342E-03 1.8364E-05 -9.7303E+04 SER
 CR                       1.9232E-03  1.0693E-01 3.0133E-03 -5.1794E+04 SER
 FE                       1.5041E-02  8.3627E-01 4.2352E-03 -4.8757E+04 SER
 NI                       8.5193E-04  4.7367E-02 1.1925E-04 -8.0610E+04 SER

 FCC_A1                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.7986E-02, Mass 1.0000E+00, Volume fraction 1.0000E+00  Mole fractions:
 FE  8.36270E-01  CR  1.06929E-01  NI  4.73667E-02  CO  9.43424E-03
POLY_3: l-st cp
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 CO                       ENTERED   SER
 CR                       ENTERED   SER
 FE                       ENTERED   SER
 NI                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    1.798594E-02
 BCC_A2#2                 ENTERED     -1.564120E-02    0.000000E+00
 BCC_A2                   ENTERED     -1.564120E-02    0.000000E+00
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1.
 N=1.7985937E-2
 N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY_3: @@
POLY_3: @@ As shown here, 1 gram of steel (Fe-10Cr-5Ni-1Co wt%)
POLY_3: @@   is equivalent to:
POLY_3: @@       n(Fe) = 1.5041094E-2
POLY_3: @@       n(Cr) = 1.9232249E-3
POLY_3: @@       n(Ni) = 8.5193389E-4
POLY_3: @@       n(Co) = 1.6968422E-4
POLY_3: @@
POLY_3:
POLY_3: @@... Saving the workspace for the Fe-Cr-Ni-Co system:
POLY_3: save TCEX53_b.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: @@ ==================================================================
POLY_3: @@ Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl system
POLY_3: @@ ******************************************************************
POLY_3: @@   Bulk composition in the heterogeneous interaction system:
POLY_3: @@          b(H2O)  = 1000
POLY_3: @@          n(NaCl) = 0.085554
POLY_3: @@          n(Fe) = 1.5041094E-2
POLY_3: @@          n(Cr) = 1.9232249E-3
POLY_3: @@          n(Ni) = 8.5193389E-4
POLY_3: @@          n(Co) = 1.6968422E-4
POLY_3:
POLY_3: @@... Retrieving data from the PAQ2 or PAQS2 database:
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_PAQ2: rej sys
   ... the command in full is REJECT
 H                        O                        ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                 DIAMOND_A4               FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                 CUB_A13                  CHI_A12
 FE4N                     FECN_CHI  REJECTED
 CEMENTITE                M23C6                    M7C3
 M5C2                     M3C2                     KSI_CARBIDE
 PI  REJECTED
 FE3C                     NI3C                     CR3C2
 CR7C3                    CR23C6  REJECTED
 COCO3                    FECO3                    NAHCO3
 NA2CO3                   NA2CO3_S2                NICO3
 CRC6O6  REJECTED
 CO3N                     CRN                      CR2N
 FE2N                     NI3N  REJECTED
 NANO2                    NANO2_S2                 NANO3
   REJECTED
 COCL2                    CRCL2                    CRCL3
 FECL2                    FECL3                    NICL2
   REJECTED
```

```
 FECLO                   NACLO4                  NACLO4_S2
   REJECTED
 REINITIATING GES5 .....
TDB_PAQ2: @@ ------ switch on PAQ2 or PAQS2
TDB_PAQ2: sw PAQ2
   ... the command in full is SWITCH_DATABASE
TDB_PAQ2: d-sys H O Na Cl Fe Cr Ni Co
   ... the command in full is DEFINE_SYSTEM
 NA                      CL                      FE
 CR                      NI                      CO
   DEFINED
TDB_PAQ2: l-sys const
   ... the command in full is LIST_SYSTEM
 AQUEOUS:A   :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CO1H2O2 CL2 CL-1 CLO2 CLO-1
  CLO2-1 CLO3-1 CLO4-1 HCLO HCLO2 CO+2 CO+3 CR+2 CR+3 CROH+2 CRO+1 CRO2-1
  HCRO2 HCRO4-1 CRO4-2 CR2O7-2 FE+2 FE+3 FEOH+1 FEOH+2 FEO3H3-1 FE2O2H2+4
  FECL+2 NA+1 NI+2 NIOH+1:
  > Aqueous Solution: using the SIT Model (from TCAQ2 database)
 REF_ELECTRODE :ZE:
  > Reference Electrode for ZE potentail; always SUSPENDED in POLY.
 GAS:G       :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1CO1 CL1CR1 CL1CR1O1
  CL1CR1O2 CL1FE1 CL1NA1 CL1NI1 CL2CO1 CL2CR1 CL2CR1O1 CL2CR1O2 CL2FE1
  CL2NA2 CL2NI1 CL3CO1 CL3CR1 CL3CR1O1 CL3FE1 CL3NA3 CL4CO2 CL4CR1 CL4CR1O1
  CL4FE2 CL5CR1 CL6CR1 CL6FE2 CO CO1H1 CO1H2O2 CO1O1 CR CR1H1 CR1H1O1
  CR1H1O2 CR1H1O3 CR1H2O2 CR1H2O3 CR1H2O4 CR1H3O3 CR1H3O4 CR1H4O4 CR1H4O5
  CR1O1 CR1O2 CR1O3 CR2 CR2O1 CR2O2 CR2O3 FE FE1H1O1 FE1H1O2 FE1H2O2 FE1O1
  FE1O2 H H1NA1 H1NA1O1 H1NI1 H1NI1O1 H1O1 H1O2 H2 H2NA2O2 H2NI1O2 H2O1 H2O2
  NA NA1O1 NA2 NA2O1 NA2O2 NI NI1O1 O O2 O3:
  > Gaseous Mixture, using the ideal gas model
 FCC_A1      :CO CR FE NA NI O:VA:
  > This is also the MX (X=C,N) solution phase.
 BCC_A2      :CO CR FE NA NI O:VA:
  > This is also the MX3 (X=C,N) solution phase.
 HCP_A3      :CO CR FE NA NI:VA:
  > This is also the M2X (X=C,N) solution phase.
 SIGMA       :CO FE NI:CR:CO CR FE NI:
 HALITE      :NA1CL1:
 WUSTITE     :FE0.947O1:
 MAGNETITE   :FE3O4:
 HEMATITE    :FE2O3:
 FE2O3_GAMMA :FE2O3:
 FEO2H2      :FE1H2O2:
 FEO3H3      :FE1H3O3:
 FEOOH       :FE1H1O2:
 FE2O2O2H2   :FE2H2O4:
 COO         :CO1O1:
 CO3O4       :CO3O4:
 COO2H2      :CO1H2O2:
 CRO2        :CR1O2:
 CRO3        :CR1O3:
 CR2O3       :CR2O3:
 CR5O12      :CR5O12:
 CR8O21      :CR8O21:
 NAO2        :NA1O2:
 NA2O        :NA2O1:
 NA2O_S2     :NA2O1:
 NA2O_S3     :NA2O1:
 NA2O2       :NA2O2:
 NA2O2_S2    :NA2O2:
 NAOH        :H1NA1O1:
 NAOH_S2     :H1NA1O1:
 NIO         :NI1O1:
 NIO_S2      :NI1O1:
 NIO2H2      :H2NI1O2:
 NIOOH       :H1NI1O2:
 FECR2O4     :CR2FE1O4:
 COCR2O4     :CO1CR2O4:
 NICR2O4     :CR2NI1O4:
 NA2CR2O4    :CR2NA2O4:
 COFE2O4     :CO1FE2O4:
 NIFE2O4     :FE2NI1O4:
 NA2CRO4     :CR1NA2O4:
 NA2CRO4_S2  :CR1NA2O4:
 NA2FEO2     :FE1NA1O2:
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: rej ph  HCP_A3 CBCC_A12 CUB_A13 CHI_A12 Fe4N
   ... the command in full is REJECT
 HCP_A3  REJECTED
TDB_PAQ2: rej ph  SIGMA
   ... the command in full is REJECT
 SIGMA  REJECTED
TDB_PAQ2: rej ph  NaH
   ... the command in full is REJECT
TDB_PAQ2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
      -Cl system.'
  'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
      -Cr-Na-Ni-C-H-O-N-S-Cl system.'
  'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
      -Na-Ni-C-H-O-N-S-Cl system.'
  'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
      only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
      from TCAQ2 which covers totally 83 elements and contains many more
      aqueous solution species.'
 -OK-
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: @@... Defining system-components and their proper reference states:
```

```
TDB_PAQ2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY_3: d-com H2O H+1 ZE Na Cl Fe Cr Ni Co
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-r-s H2O AQUEOUS * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s ZE  REF_ELE * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H2O                     ENTERED   AQUEOUS        *              100000
 H+1                     ENTERED   SER
 ZE                      ENTERED   REF_ELECTRODE  *              100000
 NA                      ENTERED   SER
 CL                      ENTERED   SER
 FE                      ENTERED   SER
 CR                      ENTERED   SER
 NI                      ENTERED   SER
 CO                      ENTERED   SER
POLY_3:
POLY_3: @@... Defining some symbols (constants/variables/functions/tables):
POLY_3: @@  ******************************************************************
POLY_3: @@  One may choose to just define some important ones as shown here,
POLY_3: @@           e.g., RNF; pH, Eh
POLY_3: @@  ==================================================================
POLY_3: @@  Important: With the default reference state (SER) used for
POLY_3: @@     system-component H+1, the pH condition in aqueous solution
POLY_3: @@     should be defined as below:
POLY_3: @@        pH = -log10[act(H+1,aqs)]                  (traditional)
POLY_3: @@           = -log10[acr(H+1,AQUEOUS)*55.508435]    (Thermo-Calc)
POLY_3: @@           = -ln[acr(H+1,AQUEOUS)*55.508435]*2.302585093
POLY_3: @@     where
POLY_3: @@       act(H+1,aqs) is molality_based activity of
POLY_3: @@           H+1 species (as of the traditional concept);
POLY_3: @@       acr(H+1,AQ)*AH2O is site-fraction_based activity of
POLY_3: @@           H+1 species (calculated in Thermo-Calc).
POLY_3: @@
POLY_3: @@     Such a definition not only gives correct pH values for all
POLY_3: @@     thermodynamic models (SIT and HKF) but also does not affect
POLY_3: @@     the calculation of ACR(H+1) [LNACR(H+1)] quantity that is
POLY_3: @@     normally used as MAPPING/STEPPING variables in all modules
POLY_3: @@     (POURBAIX & TDB/GES5/POLY3/POST).
POLY_3: @@
POLY_3: @@  ------------------------------------------------------------------
POLY_3: @@  Notes:
POLY_3: @@    If desired, one may also choose to define many other possible
POLY_3: @@      symbols (for the convenience of plotting) on the same scope
POLY_3: @@      of the POURBAIX-Module.
POLY_3: @@
POLY_3: @@    A complete list of valid symbols for the Fe-Cr-Ni-Co-H2O-NaCl
POLY_3: @@      heterogeneous interaction system on the scope same as the
POLY_3: @@      automatically-defined symbols in the POURBAIX-Module can be
POLY_3: @@      found at the end of this MACRO file (only as a reference!).
POLY_3: @@
POLY_3: @@  Please pay attention to the followings:
POLY_3: @@    * AH2O is always a constant, and YH2O is the site fraction
POLY_3: @@        of the solvent H2O, i.e.,
POLY_3: @@            AH2O = 55.508435
POLY_3: @@            YH2O = Y(AQ,H2O)
POLY_3: @@
POLY_3: @@    * The AYT and ART quantities are on the Site-Fraction basis:
POLY_3: @@            AYT for AC(i,AQ)
POLY_3: @@            ART for ACR(i,AQ)
POLY_3: @@
POLY_3: @@    * The AIT (AIi), RCT (RCi) and MLT (MLi) quantities are
POLY_3: @@        on the Molality basis:
POLY_3: @@            AIT for ACR(i,AQ)*AH2O
POLY_3: @@                  as activity based on molality
POLY_3: @@            RCT for ACR(i,AQ)*YH2O/Y(AQ,i)
POLY_3: @@                  as activity coefficient based on molality
POLY_3: @@            MLT for Y(AQ,i)*AH2O/YH2O
POLY_3: @@                  as molality
POLY_3: @@           ----------------------------------------------------
POLY_3: @@            AIi = RCi * MLi
POLY_3: @@                = ACR(i,AQ)*YH2O/Y(AQ,i) * Y(AQ,i)*AH2O/YH2O
POLY_3: @@                = ACR(i,AQ)*AH2O
POLY_3: @@
POLY_3: @@    * It is always ACR(sp,AQ) = AC(sp,AQ)
POLY_3: @@
POLY_3: @@    * It is always the AIi=AIT(H+1) [=ACR(H+1,AQ)*AH2O] quantity,
POLY_3: @@        rather than ART(H+1) [=ACR(H+1,AQ)] quantity, that is
POLY_3: @@        the equivalent property for the acidity condition pH.
POLY_3: @@  ------------------------------------------------------------------
POLY_3: @@
POLY_3: ent-sym const AH2O=55.508435
   ... the command in full is ENTER_SYMBOL
POLY_3: ent-sym const RNF =96485.309
   ... the command in full is ENTER_SYMBOL
POLY_3: ent-sym funct Eh = mur(ZE)/RNF;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent-sym funct pH = -log10(acr(H+1,AQUEOUS)*AH2O);
   ... the command in full is ENTER_SYMBOL
POLY_3: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED CONSTANTS
    AH2O=55.508435, RNF=96485.309
 DEFINED FUNCTIONS AND VARIABLES%
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
POLY_3:
POLY_3: @@... Defining the equilibrium conditions:
POLY_3: @@    ------------------------------------------------------------
POLY_3: @@     Defining P-T and bulk composition in the interaction system
POLY_3: @@     for calculating starting point [at e.g pH=7 & Eh=0 (V)]:
POLY_3: @@
POLY_3:
```

```
POLY_3: @@ ------ P-T conditions:
POLY_3: s-c P=1e5 T=298.15
   ... the command in full is SET_CONDITION
POLY_3: @@
POLY_3: @@      ... Alternatively, it can be manually input as below:
POLY_3: @@   s-c P=
POLY_3: @@ @?Pressure_in_Pascal:
POLY_3: @@   s-c T=
POLY_3: @@ @?Temperature_In_Kelvin:
POLY_3:
POLY_3: @@ ------ For Aqueous-involving interaction system, it is always
POLY_3: @@        recommended to define 1 kg of H2O, so that it is very
POLY_3: @@        convenient to consider molality quantities and other
POLY_3: @@        properties in aqueous solution.
POLY_3: s-c b(H2O)=1000
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ------ The following is equivalent to 0.085554 mole of NaCl
POLY_3: @@                                        in 1 kg of H2O:
POLY_3: s-c n(Na)=0.085554  n(Cl)=0.085554
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ------ For calculating Pourbaix diagrams or other diagrams in
POLY_3: @@        aqueous-involving interaction system, it is important
POLY_3: @@        to consider the so-called "effective interaction rate".
POLY_3: @@
POLY_3: @@     The following is equivalent to 1 gram of specified steel
POLY_3: @@        (Fe-10Cr-5Ni-1Co wt%) in an effective interaction with
POLY_3: @@        1 kg of H2O (dissolving 0.085554 mole of NaCl):
POLY_3: s-c n(Fe)=1.5041094E-2  n(Cr)=1.9232249E-3
   ... the command in full is SET_CONDITION
POLY_3: s-c n(Ni)=8.5193389E-4  n(Co)=1.6968422E-4
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ------ Let's calculate initial equilibrium at pH=7 & Eh=0 (V):
POLY_3: s-c lnacr(H+1)=-16.11809565  mur(ZE)=0
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
    LNACR(H+1)=-16.1181, MUR(ZE)=0
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: @@ ===================================================================
POLY_3: @@... Turn off GLOBAL completely for aqueous calculations!
POLY_3: @@ ------------------------------------------------------
POLY_3: @@   Adv-Opt GLOBAL
POLY_3: @@     Use global minimization as much as possible /N/: N
POLY_3: @@     Use global minimization for test only? /N/:      N
POLY_3: @@ ------------------------------------------------------
POLY_3: @@
POLY_3:    Adv-Opt GLOBAL N N !
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY_3: @@
POLY_3: @@ ------------------------------------------------------
POLY_3: @@   Adv-Opt EQ_CALC
POLY_3: @@     Force positive definite phase Hessian /Y:      N
POLY_3: @@     Control stepsize during minimization /Y:       Y
POLY_3: @@ ------------------------------------------------------
POLY_3:    Adv-Opt EQ_CALC N Y !
   ... the command in full is ADVANCED_OPTIONS
 Settings for the minimization of an equilibra:
POLY_3:
POLY_3: @@ ===================================================================
POLY_3: @@... Setting numerical limits:
POLY_3: @@  ------------------------------------------------------------------
POLY_3: @@  Notes:
POLY_3: @@    For equilibrium calculations (single-point, stepping or mapping)
POLY_3: @@      of complex aqueous-bearing heterogeneous interaction systems,
POLY_3: @@      it is recommended to properly modify the numerical limits.
POLY_3: @@    The following command (changing the numerical limits from the
POLY_3: @@      default values "500 1E-6 1E-12 N" to "20000 1E-6 1E-20 Y")
POLY_3: @@      will bring the following changes:
POLY_3: @@      1) The change on "Maximum number of iterations" from the
POLY_3: @@           default value 500 to 20000, which enforces 40 times
POLY_3: @@           more iterations for each of the calculations in order
POLY_3: @@           to obtain stable equilibria;
POLY_3: @@      2) The "Required accuracy" remains the default value 1E-6.
POLY_3: @@           It may be changed to 1E-4, that will allow less accurate
POLY_3: @@           calculations and thus make it easier/faster to converge;
POLY_3: @@      3) The change on "Smallest fraction" from the default site
POLY_3: @@           fraction of 1E-12 to 1E-20, that is more suitable for
POLY_3: @@           for aqueous solution phase; and
POLY_3: @@      4) The "Approximate driving force for metastable phases" option
POLY_3: @@           is changed from the default value of "N" to "Y" (meaning
POLY_3: @@           it should always approximately calculate driving forces
POLY_3: @@           for metastable phases).
POLY_3: @@    Such changes in the numerical limits are essential and useful
POLY_3: @@      for making sure of finding a converged solution of stable
POLY_3: @@      equlibria, especially when the heterogeneous interaction
POLY_3: @@      system becomes more and more complicated.
POLY_3: @@  ------------------------------------------------------------------
POLY_3: @@
POLY_3:    s-n-l 20000 1e-6 1e-20 Y
   ... the command in full is SET_NUMERICAL_LIMITS
 LIMITATIONS of the present version of Thermo-Calc
 Max number of elements                        :  40
 Max number of species                         :5000
 Max number of sublattices in a phase          :  10
 Max number of constituents in a phase:        : 200

 Max number of constituents in an ideal phase :5000

POLY_3:

POLY_3:
POLY_3: @@... Calculating an equilibrium with only AQUEOUS presented:
POLY_3: c-st p *=sus
```

```
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 AQUEOUS                  ENTERED      0.000000E+00    6.138000E+03
 SUSPENDED PHASES:
 WUSTITE REF_ELECTRODE NIO_S2 NIOOH NIO2H2 NIO NIFE2O4 NICR2O4 NAOH_S2 NAOH
 NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O NA2FEO2 NA2CRO4_S2 NA2CRO4 NA2CR2O4
 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4 FE2O3_GAMMA FE2O2O2H2
 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO2H2 COO COFE2O4 COCR2O4 CO3O4 BCC_A2
 GAS
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
   109 ITS,   CPU TIME USED   0 SECONDS
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
    LNACR(H+1)=-16.1181, MUR(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.57254E+01,  Mass in grams  1.00599E+03
 Total Gibbs energy -1.70641E+07,  Enthalpy -1.59024E+07,  Volume -4.21624E-08

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                      5.5508E+01  9.9611E-01 9.9606E-01 -9.7846E+00 AQUEOUS
 H+1                     -1.0027E-02 -1.7993E-04 1.0000E-07 -3.9956E+04 SER
 ZE                       3.7895E-02  6.8003E-04 1.0000E+00  0.0000E+00 REF_ELEC
 NA                       8.5554E-02  1.5353E-03 1.5211E-50 -2.8436E+05 SER
 CL                       8.5554E-02  1.5353E-03 1.1822E-30 -1.7083E+05 SER
 FE                       1.5041E-02  2.6991E-04 1.2285E-18 -1.0223E+05 SER
 CR                       1.9232E-03  3.4513E-05 1.6596E-45 -2.5561E+05 SER
 NI                       8.5193E-04  1.5288E-05 6.0058E-14 -7.5468E+04 SER
 CO                       1.6968E-04  3.0450E-06 3.2708E-16 -8.8391E+04 SER

 AQUEOUS                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.5725E+01, Mass 1.0060E+03, Volume fraction 1.0000E+00  Mole fractions:
 H2O  9.96107E-01  ZE   6.80033E-04  NI   1.52881E-05
 CL   1.53528E-03  FE   2.69915E-04  CO   3.04501E-06
 NA   1.53528E-03  CR   3.45125E-05  H+1 -1.79930E-04
 Constitution:            SiteFraction    Molality      Activity    log10Act
 H2O                       9.96604E-01   5.55084E+01   9.96157E-01    -0.0017
 CL-1                      1.53628E-03   8.55668E-02   6.59412E-02    -1.1808
 NA+1                      1.53628E-03   8.55668E-02   6.59591E-02    -1.1807
 FE+2                      1.56791E-04   8.73285E-03   3.08751E-03    -2.5104
 FEOH+1                    1.13299E-04   6.31049E-03   4.86919E-03    -2.3125
 CRO+1                     3.00740E-05   1.67505E-03   1.29247E-03    -2.8886
 NI+2                      1.52852E-05   8.51348E-04   3.02381E-04    -3.5194
 CROH+2                    3.38456E-06   1.88512E-04   6.68399E-05    -4.1750
 CO+2                      3.04698E-06   1.69710E-04   6.02711E-05    -4.2199
 HCRO2                     1.05903E-06   5.89856E-05   5.89799E-05    -4.2293
 NIOH+1                    1.28111E-08   7.13548E-07   5.50574E-07    -6.2592
 CR+3                      1.12056E-08   6.24122E-07   6.07385E-08    -7.2165
 CRO2-1                    6.16631E-09   3.43448E-07   2.65005E-07    -6.5767
 OH-1                      2.33522E-09   1.30066E-07   1.00231E-07    -6.9990
 H+1                       2.32641E-09   1.29576E-07   1.00000E-07    -7.0000
 FEOH+2                    1.10316E-12   6.14435E-11   2.17858E-11   -10.6618
 CR+2                      1.47493E-16   8.21498E-15   2.91275E-15   -14.5357
 FE+3                      6.69156E-17   3.72704E-15   3.61605E-16   -15.4418
 FECL+2                    3.43228E-17   1.91170E-15   6.77823E-16   -15.1689
 H2                        1.06276E-19   5.91933E-18   5.91876E-18   -17.2278
 FE2O2H2+4                 2.32944E-20   1.29744E-18   2.05117E-20   -19.6880
 O3                        1.00000E-20   0.00000E+00   2.0444E-113  -112.6894
 FEO3H3-1                  1.00000E-20   0.00000E+00   4.15261E-44   -43.3817
 H2O2                      1.00000E-20   0.00000E+00   3.35251E-46   -45.4746
 CRO4-2                    1.00000E-20   0.00000E+00   1.67197E-26   -25.7768
 HCLO                      1.00000E-20   0.00000E+00   2.78756E-45   -44.5548
 HCLO2                     1.00000E-20   0.00000E+00   1.00400E-87   -86.9983
 CR2O7-2                   1.00000E-20   0.00000E+00   9.28118E-52   -51.0324
 HCRO4-1                   1.00000E-20   0.00000E+00   5.05292E-27   -26.2965
 HO2-1                     1.00000E-20   0.00000E+00   7.09471E-51   -50.1491
 CO1H2O2                   1.00000E-20   0.00000E+00   5.9656E-101  -100.2243
 CO+3                      1.00000E-20   0.00000E+00   7.96270E-38   -37.0989
 O2                        1.00000E-20   0.00000E+00   2.17014E-58   -57.6635
 CLO4-1                    1.00000E-20   0.00000E+00   5.4430E-133  -132.2642
 CLO3-1                    1.00000E-20   0.00000E+00   1.0463E-105  -104.9803
 CLO2-1                    1.00000E-20   0.00000E+00   1.05079E-82   -81.9785
 CLO2                      1.00000E-20   0.00000E+00   1.1394E-100   -99.9433
 CLO-1                     1.00000E-20   0.00000E+00   6.04311E-46   -45.2187
 CL2                       1.00000E-20   0.00000E+00   3.87204E-50   -49.4121
 Solution Properties:    pH =    7.0000    Eh =    0.0000 V      I =   0.1094
                         pe =    0.0000    Ah =    0.0000 kJ   m* =   0.1891
                         Aw =    0.9962    Os =    1.1300     pKw =  13.9973
                         At1= 1.0000E-20  At2= 1.3007E-07 (equiv_mol/kg_H2O)
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 AQUEOUS                  ENTERED      0.000000E+00    5.572540E+01
 SUSPENDED PHASES:
 WUSTITE REF_ELECTRODE NIO_S2 NIOOH NIO2H2 NIO NIFE2O4 NICR2O4 NAOH_S2 NAOH
 NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O NA2FEO2 NA2CRO4_S2 NA2CRO4 NA2CR2O4
 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4 FE2O3_GAMMA FE2O2O2H2
 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO2H2 COO COFE2O4 COCR2O4 CO3O4 BCC_A2
 GAS
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.9899
 N=55.725397
 N(H2O)=55.508435, N(H+1)=-1.0026646E-2, N(ZE)=3.7895099E-2, N(NA)=8.5554E-2,
    N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
    N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY_3:Hit RETURN to continuePOLY_3:
POLY_3: @@... Calculating an equilibrium with all phases presented:
POLY_3: @@                                          (except for REF_ELE)
POLY_3: c-st p *=ent 0
```

```
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY_3: @@ ...... Always setting the REF_ELECTRODE phase as SUSPENDED:
POLY_3: c-st p REF_ELE=sus
   ... the command in full is CHANGE_STATUS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 WUSTITE                 ENTERED      0.000000E+00    0.000000E+00
 NIO_S2                  ENTERED      0.000000E+00    0.000000E+00
 NIOOH                   ENTERED      0.000000E+00    0.000000E+00
 NIO2H2                  ENTERED      0.000000E+00    0.000000E+00
 NIO                     ENTERED      0.000000E+00    0.000000E+00
 NIFE2O4                 ENTERED      0.000000E+00    0.000000E+00
 NICR2O4                 ENTERED      0.000000E+00    0.000000E+00
 NAOH_S2                 ENTERED      0.000000E+00    0.000000E+00
 NAOH                    ENTERED      0.000000E+00    0.000000E+00
 NAO2                    ENTERED      0.000000E+00    0.000000E+00
 NA2O_S3                 ENTERED      0.000000E+00    0.000000E+00
 NA2O_S2                 ENTERED      0.000000E+00    0.000000E+00
 NA2O2_S2                ENTERED      0.000000E+00    0.000000E+00
 NA2O2                   ENTERED      0.000000E+00    0.000000E+00
 NA2O                    ENTERED      0.000000E+00    0.000000E+00
 NA2FEO2                 ENTERED      0.000000E+00    0.000000E+00
 NA2CRO4_S2              ENTERED      0.000000E+00    0.000000E+00
 NA2CRO4                 ENTERED      0.000000E+00    0.000000E+00
 NA2CR2O4                ENTERED      0.000000E+00    0.000000E+00
 MAGNETITE               ENTERED      0.000000E+00    0.000000E+00
 HEMATITE                ENTERED      0.000000E+00    0.000000E+00
 HALITE                  ENTERED      0.000000E+00    0.000000E+00
 FEOOH                   ENTERED      0.000000E+00    0.000000E+00
 FEO3H3                  ENTERED      0.000000E+00    0.000000E+00
 FEO2H2                  ENTERED      0.000000E+00    0.000000E+00
 FECR2O4                 ENTERED      0.000000E+00    0.000000E+00
 FE2O3_GAMMA             ENTERED      0.000000E+00    0.000000E+00
 FE2O2O2H2               ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                  ENTERED      0.000000E+00    0.000000E+00
 CRO3                    ENTERED      0.000000E+00    0.000000E+00
 CRO2                    ENTERED      0.000000E+00    0.000000E+00
 CR8O21                  ENTERED      0.000000E+00    0.000000E+00
 CR5O12                  ENTERED      0.000000E+00    0.000000E+00
 CR2O3                   ENTERED      0.000000E+00    0.000000E+00
 COO2H2                  ENTERED      0.000000E+00    0.000000E+00
 COO                     ENTERED      0.000000E+00    0.000000E+00
 COFE2O4                 ENTERED      0.000000E+00    0.000000E+00
 COCR2O4                 ENTERED      0.000000E+00    0.000000E+00
 CO3O4                   ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                  ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS                 ENTERED      0.000000E+00    5.583623E+01
 GAS                     ENTERED      0.000000E+00    0.000000E+00
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM

    79 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
    LNACR(H+1)=-16.1181, MUR(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.56976E+01,  Mass in grams  1.00595E+03
 Total Gibbs energy -1.70627E+07,  Enthalpy -1.59010E+07,  Volume -3.10120E-16

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                     5.5508E+01  9.9660E-01 9.9654E-01 -8.5924E+00 AQUEOUS
 H+1                    -5.2910E-02 -9.4995E-04 1.0000E-07 -3.9956E+04 SER
 ZE                      5.2936E-02  9.5042E-04 1.0000E+00 -4.4035E-12 REF_ELEC
 NA                      8.5554E-02  1.5360E-03 1.5537E-50 -2.8431E+05 SER
 CL                      8.5554E-02  1.5360E-03 1.2078E-30 -1.7077E+05 SER
 FE                      1.5041E-02  2.7005E-04 5.2232E-26 -1.4431E+05 SER
 CR                      1.9232E-03  3.4530E-05 1.2572E-53 -3.0196E+05 SER
 NI                      8.5193E-04  1.5296E-05 1.0073E-15 -8.5603E+04 SER
 CO                      1.6968E-04  3.0465E-06 1.5331E-20 -1.1310E+05 SER

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5653E+01, Mass 1.0045E+03, Volume fraction 1.0000E+00  Mole fractions:
 H2O  9.96925E-01  ZE   4.72606E-07  FE   1.08577E-11
 NA   1.53727E-03  NI   2.36161E-07  CR   2.55062E-13
 CL   1.53727E-03  CO   1.31447E-10  H+1 -2.25543E-10
 Constitution:           SiteFraction    Molality      Activity    log10Act
 H2O                      9.96925E-01   5.55084E+01   9.96603E-01    -0.0015
 NA+1                     1.53727E-03   8.55948E-02   6.73703E-02    -1.1715
 CL-1                     1.53727E-03   8.55948E-02   6.73703E-02    -1.1715
 NI+2                     2.35950E-07   1.31376E-05   5.07139E-06    -5.2949
 OH-1                     2.28889E-09   1.27444E-07   1.00279E-07    -6.9988
 H+1                      2.27916E-09   1.26903E-07   1.00000E-07    -7.0000
 NIOH+1                   2.10599E-10   1.17261E-08   9.23842E-09    -8.0344
 CO+2                     1.31447E-10   7.31890E-09   2.82496E-09    -8.5490
 FE+2                     6.13590E-12   3.41645E-10   1.31278E-10    -9.8818
 FEOH+1                   4.72178E-12   2.62907E-10   2.07132E-10    -9.6838
 CRO+1                    2.23303E-13   1.24334E-11   9.79571E-12   -11.0090
 CROH+2                   2.36100E-14   1.31459E-12   5.06585E-13   -12.2953
 HCRO2                    8.03267E-15   4.47256E-13   4.47228E-13   -12.3495
 CR+3                     7.04094E-17   3.92037E-15   4.60120E-16   -15.3371
 CRO2-1                   4.58077E-17   2.55056E-15   2.00946E-15   -14.6969
 H2                       1.06307E-19   5.91913E-18   5.91876E-18   -17.2278
 FEOH+2                   4.31923E-20   2.40493E-18   9.26752E-19   -18.0330
 O2                       1.00000E-20   5.56796E-19   2.17223E-58   -57.6631
 FEO3H3-1                 1.00000E-20   5.56796E-19   1.76819E-51   -50.7525
 FECL+2                   1.00000E-20   5.56796E-19   2.94449E-23   -22.5310
 FE2O2H2+4                1.00000E-20   5.56796E-19   3.71178E-35   -34.4304
 FE+3                     1.00000E-20   5.56796E-19   1.53750E-23   -22.8132
 H2O2                     1.00000E-20   5.56796E-19   3.35574E-46   -45.4742
 HCLO                     1.00000E-20   5.56796E-19   2.84935E-45   -44.5453
 CRO4-2                   1.00000E-20   5.56796E-19   1.26903E-34   -33.8965
 HCLO2                    1.00000E-20   5.56796E-19   1.02675E-87   -86.9885
 HCRO4-1                  1.00000E-20   5.56796E-19   3.83517E-35   -34.4162
```

```
 CR2O7-2                  1.00000E-20   5.56796E-19   5.34416E-68   -67.2721
 HO2-1                    1.00000E-20   5.56796E-19   7.10153E-51   -50.1486
 CR+2                     1.00000E-20   5.56796E-19   2.20654E-23   -22.6563
 CO1H2O2                  1.00000E-20   5.56796E-19   2.7988E-105  -104.5530
 CO+3                     1.00000E-20   5.56796E-19   3.73219E-42   -41.4280
 O3                       1.00000E-20   5.56796E-19   2.0474E-113  -112.6888
 CLO4-1                   1.00000E-20   5.56796E-19   5.5717E-133  -132.2540
 CLO3-1                   1.00000E-20   5.56796E-19   1.0705E-105  -104.9704
 CLO2-1                   1.00000E-20   5.56796E-19   1.07460E-82   -81.9688
 CLO2                     1.00000E-20   5.56796E-19   1.1652E-100   -99.9336
 CLO-1                    1.00000E-20   5.56796E-19   6.17706E-46   -45.2092
 CL2                      1.00000E-20   5.56796E-19   4.04170E-50   -49.3934
 Solution Properties:   pH =   7.0000    Eh =   -0.0000 V     I =   0.0856
                        pe =  -0.0000    Ah =   -0.0000 kJ   m* =   0.1712
                        Aw =   0.9966    Os =    1.1033     pKw =  13.9973
                        At1= 1.0000E-20  At2= 1.2744E-07 (equiv_mol/kg_H2O)

 HEMATITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 3.3409E-02, Mass 1.0670E+00, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.20000E+00  NI   0.00000E+00  NA   0.00000E+00
 H2O  6.00000E-01  CR   0.00000E+00  CO   0.00000E+00
 FE   4.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00

 NIFE2O4                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.8715E-03, Mass 1.9660E-01, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.14286E+00  NI   1.42857E-01  NA   0.00000E+00
 H2O  5.71429E-01  CR   0.00000E+00  CO   0.00000E+00
 FE   2.85714E-01  CL   0.00000E+00  H+1 -1.14286E+00

 CR2O3                       Status ENTERED     Driving force  0.0000E+00
 Moles 3.9597E-03, Mass 1.2037E-01, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.20000E+00  NI   0.00000E+00  NA   0.00000E+00
 H2O  6.00000E-01  FE   0.00000E+00  CO   0.00000E+00
 CR   4.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00

 COCR2O4                     Status ENTERED     Driving force  0.0000E+00
 Moles 1.1877E-03, Mass 3.8504E-02, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.14286E+00  CO   1.42857E-01  NA   0.00000E+00
 H2O  5.71429E-01  NI   0.00000E+00  FE   0.00000E+00
 CR   2.85714E-01  CL   0.00000E+00  H+1 -1.14286E+00
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 NIFE2O4                ENTERED      0.000000E+00    5.871536E-03
 HEMATITE               ENTERED      0.000000E+00    3.340878E-02
 CR2O3                  ENTERED      0.000000E+00    3.959678E-03
 COCR2O4                ENTERED      0.000000E+00    1.187738E-03
 AQUEOUS                ENTERED      0.000000E+00    5.565313E+01
 FECR2O4                ENTERED     -1.007600E-01    0.000000E+00
 FE2O2O2H2              ENTERED     -1.872978E-01    0.000000E+00
 FEOOH                  ENTERED     -2.260402E-01    0.000000E+00
 COFE2O4                ENTERED     -8.149192E-01    0.000000E+00
 FEO3H3                 ENTERED     -1.157510E+00    0.000000E+00
 NICR2O4                ENTERED     -1.415362E+00    0.000000E+00
 FE2O3_GAMMA            ENTERED     -1.461433E+00    0.000000E+00
 MAGNETITE              ENTERED     -1.556302E+00    0.000000E+00
 NIO2H2                 ENTERED     -3.146330E+00    0.000000E+00
 NIO                    ENTERED     -4.159999E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -4.169527E+00
 NIO_S2 HALITE COO2H2 FEO2H2 NA2CR2O4 NA2FEO2 CO3O4 WUSTITE COO CRO2 NA2CRO4
 NA2CRO4_S2 NIOOH CR5O12 NAOH NAOH_S2 CR8O21 CRO3 GAS NA2O2 NA2O2_S2 NA2O
 NA2O_S2 NA2O_S3 NAO2 FCC_A1 BCC_A2
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.9467
 N=55.697555
 N(H2O)=55.508435, N(H+1)=-5.2909903E-2, N(ZE)=5.2936192E-2, N(NA)=8.5554E-2,
    N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
    N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY_3:
POLY_3: @@... Saving the workspace for the single-point equilibrium
POLY_3: @@                     of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY_3: save TCEX53_c.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continuePOLY_3:
POLY_3: @@ ================================================================
POLY_3: @@ Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl system
POLY_3: @@ ****************************************************************
POLY_3:
POLY_3: @@... Defining the mapping variables for Pourbaix-diagram mapping:
POLY_3: @@                          pH from  0   to 14
POLY_3: @@                          Eh from -1.2 to 1.5 (V)
POLY_3: s-a-v 1 lnacr(H+1) -32.22994 0 0.5
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 mur(Ze) -150000 200000 5000

   ... the command in full is SET_AXIS_VARIABLE
POLY_3: l-a-v
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: LNACR(H+1)            Min: -32.22994 Max: 0         Inc: 0.5
  Axis No 2: MUR(ZE)               Min: -150000   Max: 200000    Inc: 5000
POLY_3:
POLY_3: @@... Adding the starting points as initial equilibria:
POLY_3: @@      (they may be enforced in 2 or 4 directions with the option >)
POLY_3: @@
POLY_3:    add 1>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:    add -1>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:    add 2>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:    add -2>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: @@... One may have more starting points at other pH-Eh conditions
POLY_3: @@      [corresponding to varied lnacr(H+1) and mur(Ze) values],
POLY_3: @@      and add them as initial equilibria.
POLY_3: @@
POLY_3: @@ s-c lnacr(H+1)=-23.0
POLY_3: @@ s-c mur(ZE)=-2000
POLY_3: @@ l-c
```

```
POLY_3: @@ c-e
POLY_3: @@ l-e ,x
POLY_3: @@
POLY_3:
POLY_3:
POLY_3: li-in-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  +1> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
    N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
 No 2  -1> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
    N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
 No 3  +2> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
    N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
 No 4  -2> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
    N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
POLY_3:
POLY_3: @@... Saving the workspace for the Pourbaix-diagram settings
POLY_3: @@                   of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY_3: save TCEX53_d.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continuePOLY_3:
POLY_3: @@... Performing the mapping calculation:
POLY_3: @@    -------------------------------------------------------------
POLY_3: @@    Due to the complexity of aqueous solution model (SIT or HKF),
POLY_3: @@    a complete mapping calculation of the Pourbaix-diagram type
POLY_3: @@    may take a rather long time. Please be patient...
POLY_3: @@    -------------------------------------------------------------
POLY_3: MAP
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12

 Phase region boundary   1 at:  -1.541E+01 -4.404E-12
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated..                      35  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:  -3.223E+01 -4.165E+04
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated.                      38  equilibria

 Phase region boundary   3 at:  -1.404E+01  3.415E+03
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
  ** NIFE2O4

 Phase region boundary   4 at:  -1.404E+01  3.415E+03
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
 Calculated.                       7  equilibria

 Phase region boundary   5 at:  -1.110E+01  1.070E+04
     AQUEOUS
  ** COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE

 Phase region boundary   6 at:  -1.110E+01  1.070E+04
     AQUEOUS
     CR2O3
  ** FECR2O4
     HEMATITE
 Calculated.                       8  equilibria

 Phase region boundary   7 at:  -7.729E+00  1.905E+04
     AQUEOUS
     CR2O3
  ** FECR2O4
  ** HEMATITE

 Phase region boundary   8 at:  -7.729E+00  1.905E+04
     AQUEOUS
     CR2O3
  ** FECR2O4
 Calculated.                       9  equilibria
```

```
Phase region boundary   9 at:  -7.729E+00 -1.955E+04
 ** GAS
    AQUEOUS
    CR2O3
 ** FECR2O4

Phase region boundary  10 at:  -7.729E+00 -1.955E+04
    GAS
    AQUEOUS
    CR2O3
 ** FECR2O4
Calculated.                      3  equilibria

Phase region boundary  11 at:  -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
 ** CR2O3
 ** FECR2O4

Phase region boundary  12 at:  -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
 ** FECR2O4
Calculated                     44  equilibria

Phase region boundary  13 at:  -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
 ** CR2O3
Calculated.                      2  equilibria

Phase region boundary  14 at:  -7.259E+00 -1.839E+04
 ** GAS
    AQUEOUS
 ** CR2O3

Phase region boundary  15 at:  -7.259E+00 -1.839E+04
    AQUEOUS
 ** CR2O3
Calculated.                     10  equilibria

Phase region boundary  16 at:  -7.259E+00  2.259E+04
    AQUEOUS
 ** CR2O3
 ** HEMATITE

Phase region boundary  17 at:  -7.259E+00  2.259E+04
    AQUEOUS
 ** CR2O3
    HEMATITE
Calculated.                     32  equilibria

Phase region boundary  18 at:  -1.110E+01  7.654E+04
    AQUEOUS
 ** COCR2O4
 ** CR2O3
    HEMATITE

Phase region boundary  19 at:  -1.110E+01  7.654E+04
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
Calculated.                      7  equilibria

Phase region boundary  20 at:  -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
 ** NIFE2O4

Phase region boundary  21 at:  -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
    NIFE2O4
Calculated..                     38  equilibria
Terminating at axis limit.

Phase region boundary  22 at:  -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                      1  equilibria

Phase region boundary  23 at:  -1.404E+01  6.733E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
 ** NIFE2O4

Phase region boundary  24 at:  -1.404E+01  6.733E+04
    AQUEOUS
    CO3O4
    COCR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                      2  equilibria

Phase region boundary  25 at:  -1.404E+01  6.745E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
    HEMATITE
 ** NIFE2O4

Phase region boundary  26 at:  -1.404E+01  6.745E+04
    AQUEOUS
    CO3O4
    HEMATITE
 ** NIFE2O4
Calculated.                      5  equilibria
```

```
Phase region boundary  27 at:  -1.404E+01  8.332E+04
 ** GAS
    AQUEOUS
    CO3O4
    HEMATITE
 ** NIFE2O4

Phase region boundary  28 at:  -1.404E+01  8.332E+04
    GAS
    AQUEOUS
    CO3O4
    HEMATITE
 ** NIFE2O4
Calculated.                      11  equilibria

Phase region boundary  29 at:  -1.257E+01  8.794E+04
    GAS
    AQUEOUS
    CO3O4
 ** HALITE
    HEMATITE
 ** NIFE2O4

Phase region boundary  30 at:  -1.257E+01  8.794E+04
    GAS
    AQUEOUS
    CO3O4
    HALITE
    HEMATITE
 ** NIFE2O4
Calculated                      33  equilibria

Phase region boundary  31 at:  -1.257E+01  8.794E+04
    GAS
    AQUEOUS
    CO3O4
 ** HALITE
    HEMATITE
Calculated.                       9  equilibria

Phase region boundary  32 at:  -8.749E+00  9.740E+04
    GAS
    AQUEOUS
 ** CO3O4
 ** HALITE
    HEMATITE

Phase region boundary  33 at:  -8.749E+00  9.740E+04
    GAS
    AQUEOUS
 ** HALITE
    HEMATITE
Calculated.                      18  equilibria

Phase region boundary  34 at:  -1.463E+00  1.159E+05
    GAS
    AQUEOUS
 ** HALITE
 ** HEMATITE

Phase region boundary  35 at:  -1.463E+00  1.159E+05
    GAS
    AQUEOUS
 ** HALITE
Calculated                      52  equilibria

Phase region boundary  36 at:  -1.463E+00  1.159E+05
    GAS
    AQUEOUS
 ** HEMATITE
Calculated                       5  equilibria

Phase region boundary  37 at:  -1.463E+00  1.159E+05
    GAS
    AQUEOUS
    HALITE
 ** HEMATITE
Calculated                      27  equilibria

Phase region boundary  38 at:  -8.749E+00  9.740E+04
    GAS
    AQUEOUS
 ** CO3O4
    HEMATITE
Calculated.                       8  equilibria

Phase region boundary  39 at:  -1.021E+01  9.281E+04
 ** GAS
    AQUEOUS
 ** CO3O4
    HEMATITE

Phase region boundary  40 at:  -1.021E+01  9.281E+04
    AQUEOUS
 ** CO3O4
    HEMATITE
Calculated.                       5  equilibria

Phase region boundary  41 at:  -1.211E+01  7.398E+04
    AQUEOUS
 ** CO3O4
 ** COCR2O4
    HEMATITE

Phase region boundary  42 at:  -1.211E+01  7.398E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
Calculated.                       5  equilibria
Terminating at known equilibrium

Phase region boundary  43 at:  -1.211E+01  7.398E+04
    AQUEOUS
 ** COCR2O4
```

```
    HEMATITE
Calculated.                        4  equilibria
Terminating at known equilibrium

Phase region boundary  44 at:  -1.211E+01  7.398E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
    HEMATITE
Calculated.                        5  equilibria
Terminating at known equilibrium

Phase region boundary  45 at:  -1.021E+01  9.281E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                       20  equilibria

Phase region boundary  46 at:  -1.208E+00  1.151E+05
 ** GAS
    AQUEOUS
 ** HEMATITE

Phase region boundary  47 at:  -1.208E+00  1.151E+05
 ** GAS
    AQUEOUS
Calculated..                        4  equilibria
Terminating at axis limit.

Phase region boundary  48 at:  -1.208E+00  1.151E+05
    AQUEOUS
 ** HEMATITE
Calculated.                       28  equilibria
Terminating at known equilibrium

Phase region boundary  49 at:  -1.208E+00  1.151E+05
    GAS
    AQUEOUS
 ** HEMATITE
Calculated                       24  equilibria

Phase region boundary  50 at:  -1.021E+01  9.281E+04
 ** GAS
    AQUEOUS
    CO3O4
    HEMATITE
Calculated.                        9  equilibria
Terminating at known equilibrium

Phase region boundary  51 at:  -8.749E+00  9.740E+04
    GAS
    AQUEOUS
 ** CO3O4
    HALITE
    HEMATITE
Calculated                       39  equilibria

Phase region boundary  52 at:  -1.257E+01  8.794E+04
    GAS
    AQUEOUS
    CO3O4
 ** HALITE
    HEMATITE
    NIFE2O4
Calculated..                       41  equilibria
Terminating at axis limit.

Phase region boundary  53 at:  -1.404E+01  8.332E+04
 ** GAS
    AQUEOUS
    CO3O4
    HEMATITE
    NIFE2O4
Calculated..                       38  equilibria
Terminating at axis limit.

Phase region boundary  54 at:  -1.404E+01  6.745E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
    HEMATITE
    NIFE2O4
Calculated.                       27  equilibria

Phase region boundary  55 at:  -2.249E+01  3.456E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
 ** COFE2O4
    HEMATITE
    NIFE2O4

Phase region boundary  56 at:  -2.249E+01  3.456E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
    COFE2O4
    HEMATITE
    NIFE2O4

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Phase region boundary  57 at:  -2.249E+01  3.456E+04
    AQUEOUS
    CO3O4
 ** COFE2O4
    HEMATITE
    NIFE2O4
Calculated..                       21  equilibria
Terminating at axis limit.

Phase region boundary  58 at:  -2.249E+01  3.456E+04
    AQUEOUS
    CO3O4
    COCR2O4
 ** COFE2O4
```

```
    HEMATITE
    NIFE2O4
Calculated.                      2  equilibria

Phase region boundary  59 at:  -2.239E+01  3.480E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
 ** COFE2O4
    HEMATITE
    NIFE2O4

Phase region boundary  60 at:  -2.239E+01  3.480E+04
    AQUEOUS
    COCR2O4
 ** COFE2O4
    HEMATITE
    NIFE2O4
Calculated..                     21  equilibria
Terminating at axis limit.

Phase region boundary  61 at:  -2.239E+01  3.480E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.                     18  equilibria
Terminating at known equilibrium

Phase region boundary  62 at:  -2.239E+01  3.480E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    COFE2O4
    HEMATITE
    NIFE2O4
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  63 at:  -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
    CR2O3
    HEMATITE
 ** NIFE2O4
Calculated.                     14  equilibria
Terminating at known equilibrium

Phase region boundary  64 at:  -1.110E+01  7.654E+04
    AQUEOUS
 ** COCR2O4
    CR2O3
    HEMATITE
Calculated.                     15  equilibria
Terminating at known equilibrium

Phase region boundary  65 at:  -7.259E+00  2.259E+04
    AQUEOUS
    CR2O3
 ** HEMATITE
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  66 at:  -7.259E+00 -1.839E+04
 ** GAS
    AQUEOUS
Calculated..                     16  equilibria
Terminating at axis limit.

Phase region boundary  67 at:  -7.259E+00 -1.839E+04
 ** GAS
    AQUEOUS
    CR2O3
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary  68 at:  -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
 ** CR2O3
    FECR2O4
Calculated.                      3  equilibria

Phase region boundary  69 at:  -7.752E+00 -1.961E+04
 ** GAS
    AQUEOUS
 ** CR2O3
    FECR2O4

Phase region boundary  70 at:  -7.752E+00 -1.961E+04
    AQUEOUS
 ** CR2O3
    FECR2O4
Calculated.                      9  equilibria

Phase region boundary  71 at:  -7.752E+00  1.899E+04
    AQUEOUS
 ** CR2O3
    FECR2O4
 ** HEMATITE

Phase region boundary  72 at:  -7.752E+00  1.899E+04
    AQUEOUS
 ** CR2O3
    FECR2O4
    HEMATITE
Calculated.                      8  equilibria
Terminating at known equilibrium

Phase region boundary  73 at:  -7.752E+00  1.899E+04
    AQUEOUS
    FECR2O4
 ** HEMATITE
Calculated.                     16  equilibria
```

```
Phase region boundary  74 at:  -1.286E+01 -1.893E+04
    AQUEOUS
    FECR2O4
 ** HEMATITE
 ** MAGNETITE

Phase region boundary  75 at:  -1.286E+01 -1.893E+04
    AQUEOUS
    FECR2O4
 ** HEMATITE
    MAGNETITE
Calculated.                       4  equilibria

Phase region boundary  76 at:  -1.395E+01 -2.164E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
 ** HEMATITE
    MAGNETITE

Phase region boundary  77 at:  -1.395E+01 -2.164E+04
    AQUEOUS
    COFE2O4
    FECR2O4
 ** HEMATITE
    MAGNETITE
Calculated.                       2  equilibria

Phase region boundary  78 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
 ** HEMATITE
    MAGNETITE
 ** NIFE2O4

Phase region boundary  79 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
 ** HEMATITE
    MAGNETITE
    NIFE2O4
Calculated..                      38  equilibria
Terminating at axis limit.

Phase region boundary  80 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    MAGNETITE
 ** NIFE2O4
Calculated.                       5  equilibria

Phase region boundary  81 at:  -1.555E+01 -3.682E+04
    AQUEOUS
 ** BCC_A2
    COFE2O4
    FECR2O4
    MAGNETITE
 ** NIFE2O4

Phase region boundary  82 at:  -1.555E+01 -3.682E+04
    AQUEOUS
    BCC_A2
    COFE2O4
    FECR2O4
    MAGNETITE
 ** NIFE2O4
Calculated..                      35  equilibria
Terminating at axis limit.

Phase region boundary  83 at:  -1.555E+01 -3.682E+04
    AQUEOUS
 ** BCC_A2
    COFE2O4
    FECR2O4
    MAGNETITE
Calculated.                       2  equilibria

Phase region boundary  84 at:  -1.548E+01 -3.681E+04
    AQUEOUS
 ** BCC_A2
 ** COFE2O4
    FECR2O4
    MAGNETITE

Phase region boundary  85 at:  -1.548E+01 -3.681E+04
    AQUEOUS
 ** BCC_A2
    FECR2O4
    MAGNETITE
Calculated.                       4  equilibria

Phase region boundary  86 at:  -1.473E+01 -3.690E+04
 ** GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
    MAGNETITE

Phase region boundary  87 at:  -1.473E+01 -3.690E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
    MAGNETITE
Calculated.                       7  equilibria

Phase region boundary  88 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
 ** MAGNETITE
```

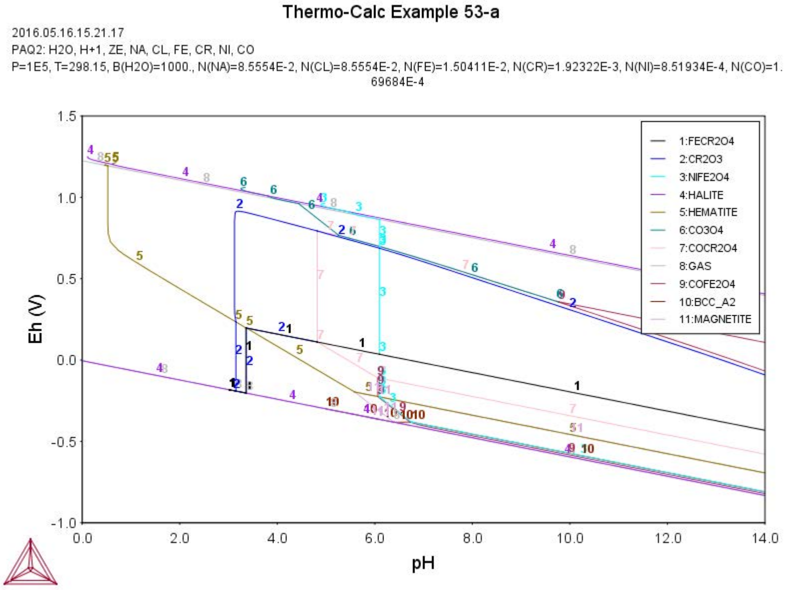
```
Phase region boundary  89 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
Calculated.                      8  equilibria

Phase region boundary  90 at:  -1.280E+01 -3.214E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
 ** HALITE

Phase region boundary  91 at:  -1.280E+01 -3.214E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
    HALITE
Calculated                    201  equilibria

Phase region boundary  92 at:  -1.280E+01 -3.214E+04
    GAS
    AQUEOUS
    FECR2O4
 ** HALITE
Calculated.                     14  equilibria

Phase region boundary  93 at:  -7.005E+00 -1.778E+04
    GAS
    AQUEOUS
 ** FECR2O4
 ** HALITE

Phase region boundary  94 at:  -7.005E+00 -1.778E+04
    GAS
    AQUEOUS
 ** HALITE
Calculated..                     16  equilibria
Terminating at axis limit.

Phase region boundary  95 at:  -7.005E+00 -1.778E+04
    GAS
    AQUEOUS
 ** FECR2O4

                                                    +                                                    ++

Phase region boundary  96 at:  -7.005E+00 -1.778E+04
    GAS
    AQUEOUS
 ** FECR2O4
    HALITE
Calculated                     62  equilibria

Phase region boundary  97 at:  -1.280E+01 -3.214E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** HALITE
Calculated.                      6  equilibria

Phase region boundary  98 at:  -1.381E+01 -3.464E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** HALITE
 ** MAGNETITE

Phase region boundary  99 at:  -1.381E+01 -3.464E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** HALITE
    MAGNETITE
Calculated..                     38  equilibria
Terminating at axis limit.

Phase region boundary 100 at:  -1.381E+01 -3.464E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** MAGNETITE

                                                    +                                                    ++

Phase region boundary 101 at:  -1.381E+01 -3.464E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
    HALITE
 ** MAGNETITE
Calculated                     61  equilibria

Phase region boundary 102 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
    FECR2O4
 ** MAGNETITE
Calculated.                      3  equilibria

Phase region boundary 103 at:  -1.472E+01 -3.688E+04
 ** GAS
    AQUEOUS
    FECR2O4
 ** MAGNETITE

Phase region boundary 104 at:  -1.472E+01 -3.688E+04
    AQUEOUS
    FECR2O4
```

```
 ** MAGNETITE
Calculated.                       5  equilibria
Terminating at known equilibrium

Phase region boundary 105 at:  -1.472E+01 -3.688E+04
 ** GAS
    AQUEOUS
    FECR2O4
Calculated.                      15  equilibria
Terminating at known equilibrium

Phase region boundary 106 at:  -1.472E+01 -3.688E+04
 ** GAS
    AQUEOUS
    FECR2O4
    MAGNETITE
Calculated.                       2  equilibria
Terminating at known equilibrium

Phase region boundary 107 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** MAGNETITE
Calculated                      46  equilibria

Phase region boundary 108 at:  -1.473E+01 -3.690E+04
 ** GAS
    AQUEOUS
    BCC_A2
    FECR2O4
    MAGNETITE
Calculated..                      38  equilibria
Terminating at axis limit.

Phase region boundary 109 at:  -1.548E+01 -3.681E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
    MAGNETITE
Calculated.                       5  equilibria
Terminating at known equilibrium

Phase region boundary 110 at:  -1.548E+01 -3.681E+04
    AQUEOUS
    BCC_A2
 ** COFE2O4
    FECR2O4
    MAGNETITE
Calculated..                      37  equilibria
Terminating at axis limit.

Phase region boundary 111 at:  -1.555E+01 -3.682E+04
    AQUEOUS
 ** BCC_A2
    COFE2O4
    FECR2O4
    MAGNETITE
    NIFE2O4
Calculated..                      35  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 112 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
    MAGNETITE
 ** NIFE2O4
Calculated.                       1  equilibria

Phase region boundary 113 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
 ** MAGNETITE
 ** NIFE2O4

Phase region boundary 114 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                       4  equilibria

Phase region boundary 115 at:  -1.404E+01 -1.073E+04
    AQUEOUS
 ** COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
 ** NIFE2O4

Phase region boundary 116 at:  -1.404E+01 -1.073E+04
    AQUEOUS
    COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                       1  equilibria
Terminating at known equilibrium

Phase region boundary 117 at:  -1.404E+01 -1.073E+04
    AQUEOUS
 ** COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
Calculated.                       2  equilibria

Phase region boundary 118 at:  -1.395E+01 -1.051E+04
```

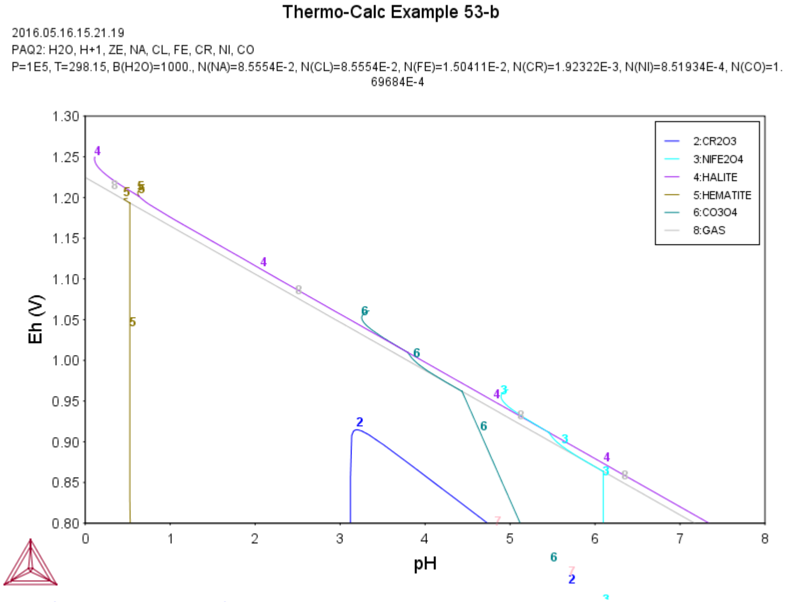
```
    AQUEOUS
 ** COCR2O4
 ** COFE2O4
    FECR2O4
    HEMATITE

Phase region boundary 119 at:  -1.395E+01 -1.051E+04
    AQUEOUS
 ** COCR2O4
    FECR2O4
    HEMATITE
Calculated.                      7  equilibria
Terminating at known equilibrium

Phase region boundary 120 at:  -1.395E+01 -1.051E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
    HEMATITE
Calculated.                      3  equilibria

Phase region boundary 121 at:  -1.395E+01 -2.164E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
    HEMATITE
 ** MAGNETITE

Phase region boundary 122 at:  -1.395E+01 -2.164E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
    HEMATITE
    MAGNETITE
Calculated.                      1  equilibria
Terminating at known equilibrium

Phase region boundary 123 at:  -1.395E+01 -2.164E+04
    AQUEOUS
    FECR2O4
    HEMATITE
 ** MAGNETITE
Calculated.                      4  equilibria
Terminating at known equilibrium

Phase region boundary 124 at:  -1.395E+01 -2.164E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
 ** MAGNETITE
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary 125 at:  -1.395E+01 -1.051E+04
    AQUEOUS
    COCR2O4
 ** COFE2O4
    FECR2O4
    HEMATITE
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary 126 at:  -1.404E+01 -1.073E+04
    AQUEOUS
 ** COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
    NIFE2O4
Calculated..                     38  equilibria
Terminating at axis limit.

Phase region boundary 127 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
 ** MAGNETITE
    NIFE2O4
Calculated..                     38  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 128 at:  -7.752E+00  1.899E+04
    AQUEOUS
    CR2O3
    FECR2O4
 ** HEMATITE
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary 129 at:  -7.752E+00 -1.961E+04
 ** GAS
    AQUEOUS
    CR2O3
    FECR2O4
Calculated.                      2  equilibria
Terminating at known equilibrium

Phase region boundary 130 at:  -1.110E+01  1.070E+04
    AQUEOUS
 ** COCR2O4
    CR2O3
    FECR2O4
    HEMATITE
Calculated.                      1  equilibria
Terminating at known equilibrium

Phase region boundary 131 at:  -1.404E+01  3.415E+03
    AQUEOUS
    COCR2O4
    CR2O3
    FECR2O4
    HEMATITE
 ** NIFE2O4
```

```
 Calculated.                        1  equilibria
 Terminating at known equilibrium

 Phase region boundary 132 at:  -1.541E+01 -4.404E-12
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated.                        4  equilibria
 Terminating at known equilibrium

 Phase region boundary 133 at:  -3.020E+01 -4.404E-12
     AQUEOUS
     COCR2O4
  ** CR2O3
     HEMATITE
     NIFE2O4
 Calculated..                        9  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 134 at:  -3.020E+01 -4.404E-12
     AQUEOUS
     COCR2O4
  ** CR2O3
     HEMATITE
     NIFE2O4
 Calculated.                       54  equilibria
 Terminating at known equilibrium

 Phase region boundary 135 at:  -1.610E+01  5.964E+04
     AQUEOUS
  ** CO3O4
     COCR2O4
     HEMATITE
     NIFE2O4
 Calculated.                       21  equilibria
 Terminating at known equilibrium

 Phase region boundary 136 at:  -1.610E+01  5.964E+04
     AQUEOUS
  ** CO3O4
     COCR2O4
     HEMATITE
     NIFE2O4
 Calculated.                        7  equilibria
 Terminating at known equilibrium

 Phase region boundary 137 at:  -1.612E+01  5.959E+04
     AQUEOUS
  ** CO3O4
     COCR2O4
     HEMATITE
     NIFE2O4
 Calculated.                       14  equilibria
 Terminating at known equilibrium

 Phase region boundary 138 at:  -1.612E+01  5.959E+04
     AQUEOUS
  ** CO3O4
     COCR2O4
     HEMATITE
     NIFE2O4
 Calculated.                        6  equilibria
 Terminating at known equilibrium

 Phase region boundary 139 at:  -1.612E+01  5.825E+04
     AQUEOUS
     COCR2O4
  ** CR2O3
     HEMATITE
     NIFE2O4
 Calculated..                       34  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 140 at:  -1.612E+01  5.825E+04
     AQUEOUS
     COCR2O4
  ** CR2O3
     HEMATITE
     NIFE2O4
 Calculated.                        6  equilibria
 Terminating at known equilibrium

 Phase region boundary 141 at:  -1.612E+01 -1.748E+03
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated..                       34  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary 142 at:  -1.612E+01 -1.748E+03
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated.                        6  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE:
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex53\TCEX
 53_d.POLY3
 CPU time for mapping                   926  seconds
POLY_3:
POLY_3: @@... Plotting the calculated Pourbaix diagram (& many others):
POLY_3: @@    ------------------------------------------------------------
POLY_3: post
```

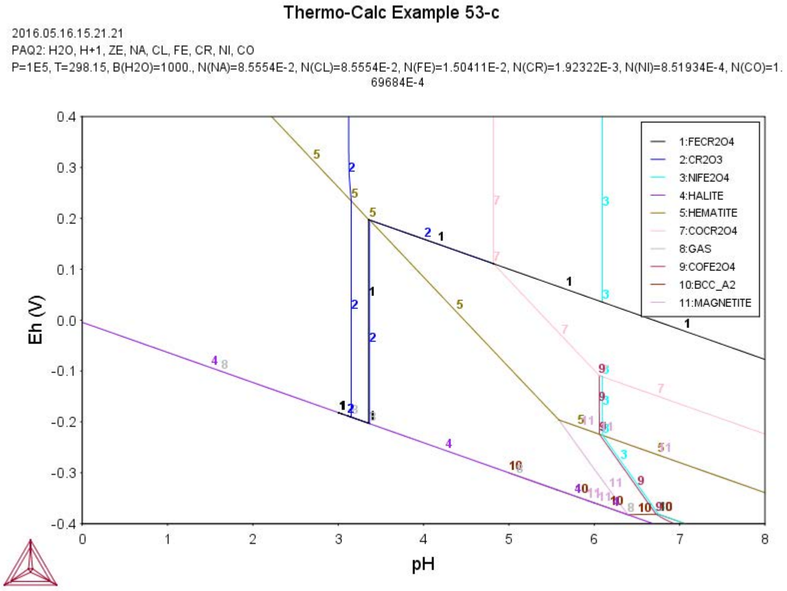
```
  POLY-3 POSTPROCESSOR VERSION 3.2


 Setting automatic diagram axes

POST: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED CONSTANTS
    AH2O=55.508435, RNF=96485.309, ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
    TEMP_C=T-273.15
POST:Hit RETURN to continuePOST:
POST: s-d-a x pH
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n pH
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:

POST: s-d-a y Eh
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text y n Eh (V)
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-t-m-s y
   ... the command in full is SET_TRUE_MANUAL_SCALING
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: s-l-c e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: s-s-s x n 0 14
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n -1.0 1.5
   ... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-a
   ... the command in full is SET_TITLE
POST: pl,,,
   ... the command in full is PLOT_DIAGRAM
```



```
POST: make TCEX53.EXP y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:Hit RETURN to continue
POST:
POST: s-s-s x n 0 8
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n .8 1.3
   ... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-b
   ... the command in full is SET_TITLE
POST:
POST: pl,,,
   ... the command in full is PLOT_DIAGRAM
```



```
POST:Hit RETURN to continue
POST:
POST: s-s-s y n -.4 .4
   ... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-c
   ... the command in full is SET_TITLE
POST:
POST: pl,,,
   ... the command in full is PLOT_DIAGRAM
```



```
POST:Hit RETURN to continue
POST:
POST: @@
POST: @@ ***********************************************************************
POST: @@ From the same mapping calculations, one may plot many more diagrams,
POST: @@    using various X-Y axis variables (for such purposes, it is very
POST: @@    convenient to use pre-defined symbols as listed at the end of
POST: @@    this MACRO file).
POST: @@ ***********************************************************************
POST: @@
POST:
POST: SET-INTERACTIVE
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

Pourbaix Diagrams

Educational Material

Thermo-Calc Software

Introduction to Pourbaix Diagrams

In this section:

About Pourbaix Diagrams in Thermo-Calc

This guide is for Thermo-Calc software users who know the basics of thermodynamics and want to know more about *Pourbaix Diagrams* below.

You are introduced to the concept of a Pourbaix diagram and shown how to interpret such diagrams through a series of examples.

Materials corrosion occurs almost everywhere. It may lead to serious material damages, unexpected application failures, tremendous economic costs and environmental degradations. Consequently, scientists and engineers must often conduct expensive and time-consuming corrosion experiments as part of failure analyses, risk evaluations, quality improvements and application enhancements.

Under certain conditions, when a metal or alloy is exposed to an aqueous solution with a concentration of inorganic/organic mixture, corrosion phenomena occur at a corresponding degree. During corrosion, some metallic phases dissolve, the metal or alloy surface gets damaged and some secondary solid phases form at the solid-liquid interfaces (such as oxides, hydroxides, silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates, or halides). Such corrosive chemical or electrochemical reactions can be studied by means of the so-called Pourbaix diagrams if the reactions reach their equilibrium states (Pourbaix, 1973, 1974; Cramer and Covino, 2003; Verink, 2011; Thompson et al., 2011).

Pourbaix Diagrams

Marcel Pourbaix applied thermodynamics to predict materials corrosion resistance. He determined the phase stability relations in terms of varied pH and Eh values for an interaction system of metal and pure water or dilute aqueous solution. He presented the stability regions of metal and secondary phases (such as metal-oxides/hydroxides) on a pH-Eh diagram, which is now known as a Pourbaix diagram.

A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). An aqueous solution phase is always present in such a system. At a given pH and Eh, a metal may lose its stability to a soluble or corrosive aqueous solution, or be in equilibrium with either the aqueous solution (insoluble/immune) or with a secondary-phase file that has formed (consisting of oxides, hydroxides, sulphides or other solids). In the latter case, further dissolution of the passive or protective metal is prevented.

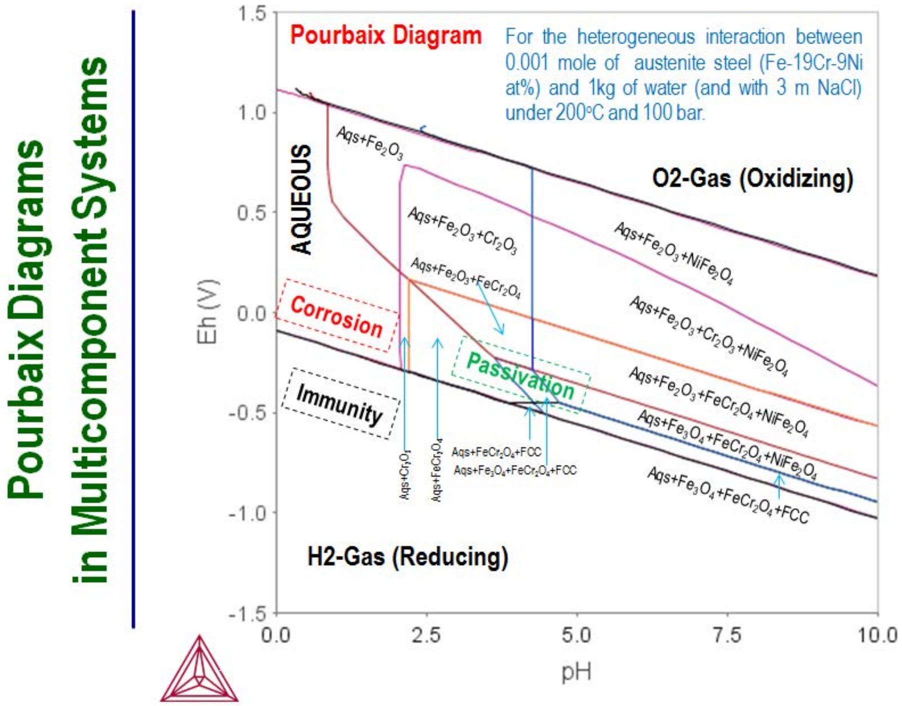
The speciation and partition in the aqueous solution and the interacting phases depend not only on pH and Eh, but also on other factors such as the bulk composition, temperature and pressure in the system. The interacting phases may be gas mixtures, stoichiometric solids or solid solutions.

A Pourbaix diagram is divided in regions of *immunity*, *corrosion* and *passivity*. These regions provides information about the stability of a particular metal or alloy in a specific aqueous electrochemical environment under certain pH, Eh, pressure and temperature conditions.

- The immunity region is the region in which there is no metal dissolution.
- The corrosion region is the region in which there is active metal dissolution.

- The passivation region is the region in which a protective metal-oxide film that prevents metal dissolution is formed.

The following shows these three regions in a Pourbaix diagram for the heterogeneous interaction between 0.001 mole of austenite steel (Fe-19Cr-9Ni [at%]) and 1 kg of water (with 3 m NaCl), at 200°C and 100 bar:



Depending on the system's bulk chemical composition, secondary phases may form during the transformation process. These can not only be oxides, but also be, for example, hydroxides, sulphides, sulphates, carbonates, nitrates, phosphates, borates, silicates, hydrous silicates and halides. Information about these secondary phases may help one understand the passivation behaviours in corrosion processes. For example, it may be important to understand whether any secondary phases are formed in different pH-Eh regions during hydrolysis, oxidation, reduction or other reaction processes.

In a Pourbaix diagram, the predominant ion boundaries are often represented by dashed and straight lines imposed on a traditional Pourbaix diagram for a simple interaction system (Pourbaix, 1973, 1974; Cramer and Covino, 2003; Verink, 2011; Thompson et al., 2011). Such a predominance boundary is normally an equal molality (or equal activity) line for a pair of two most-concentrated aqueous solute species (charged or neutral) involving a common metal. A line is then simply determined by a reaction constant of its corresponding electrochemical reaction in the homogeneous aqueous solution phase. However, this is not the case in Thermo-Calc.

You cannot get any information about predominant ion boundaries from a Pourbaix diagram in Thermo-Calc.

Working with Pourbaix Diagrams

With the Thermo-Calc software package, Pourbaix diagrams can be calculated over a wide range of pressure, temperature and composition conditions for complex heterogeneous interactions between multicomponent primary alloy solution or compound phases, concentrated aqueous solutions (with dissolved inorganic and organic substances), complicated secondary solids and oxidizing/reducing gaseous mixtures. In the Console Mode, diagrams can be calculated and plotted either using the response-driven POURBAIX module or directly using the DATA, GIBBS, POLY and POST modules.

Note that it is possible in Thermo-Calc to set aqueous properties other than pH and Eh as axis variables. For example, the following properties can also be set as axis variables: `Ah` (electronic affinity), `pe` (electronic activity log10ACRe), `IS` (ionic strength), `TM` (total aqueous concentration, in molality), `OC` (Osmotic coefficient), activity or activity coefficient of solvent H2O, and activities or activity coefficients or concentrations in m (molality) of charged or neutral solute species.

Beside a concentrated aqueous solution phase handled by a proper thermodynamic model named SIT, HKF or PITZ, it is also possible to consider complex alloy solution phases or compound phases, as well as secondary solid phases and gaseous mixtures, which are treated by specific solution models.

Most frequently, a Poubaix diagram is calculated for a specific alloyed phase with the initial alloying composition, such as the FCC solution phase in an austenite steel. However, it is possible to calculate a Pourbaix diagram for two co-existing phases, such as the FCC+BCC solution phases in a duplex steel for example, or even for more than two co-existing phases in a steel/alloy.

Note that each point on the lines in a pH-Eh diagram in Thermo-Calc represents a certain minimum state of Gibbs energy. When a line is crossed, a phase transformation should occur. This means that a Pourbaix diagram in Thermo-Calc does not provide any information about any predominant ion boundary.

Key Concepts

The following are two key concepts important for understanding how aqueous solutions behave and how an aqueous-bearing heterogeneous interaction system is properly defined and calculated in Thermo-Calc.

Effective Interaction Ratio

A pH-Eh plot is always related to a certain amount of initial alloys or other condensed materials that has effectively reacted with an aqueous solution in the system. This is the amount of condensed material that is fully in equilibrium with the defined aqueous solution phase. The amount is specified relative to an aqueous solution that is normally comprised of 1 kg of water with certain specified solute concentrations at certain temperature and pressure conditions. (This is why a calculated Pourbaix diagram is typically presented for an initial amount of the interacting metal or alloy at a certain level, such as 10-6, 1E-3, 0.1 or 1 mole of metal or alloy.) It is called the *Effective Interaction Ratio* (between the initial alloy or alloyed phases and the initial aqueous solution) and it is expressed in terms of molality (mol/kg).

The Effective Interaction Ratio is important for two reasons. First, the ratio has implications for kinetic or dynamic effects such as chemical reaction mechanism and kinetics, fluid flow dynamics, surface area and interaction time. Secondly, the ratio, being expressed as 10-6 mole of metal (or alloy), is the solubility limit that can be detected for cathodic corrosion protection by immunity.

One should always be careful when setting initial amounts and compositions in the original condensed materials, as well as when setting the initial concentrations of dissolved solutes in the original aqueous solution phase. It is often useful to make a series of calculations for different levels of initial amount of the interacting metal/alloy while the conditions are fixed for other settings (such as initial aqueous concentration, pressure, temperature, pH, and Eh).

Solubility

When a heterogeneous equilibrium has a dissolving solution or mixture phase and a stoichiometric or solution phase, then the concept of solubility becomes important. A solubility of a phase (the solute) is its property of dissolving in the solvent phase. This concept concerns the constitution of a phase and is applied where one or several of the constituents are dominant (which is highly concentrated and dissolving) while there are only small amounts of the other remaining species (which are less concentrated and dissolved). The dissolving solution or mixture phase can be liquid, gas, aqueous or solid, as long as it has dissolving capacity. The stoichiometric or solution phase has some constituents which tend to be dissolved into the dissolving solution or mixture phase.

Key Points about Solubility

- Under certain temperature, pressure and composition conditions, a Fe- or Cr-dominant BCC phase can dissolve certain amounts of Ni and C from a carbide phase such as M23C6, M7C3 or M3C. The Ni and C elements in the carbides have the solubility defined relative to the BCC phase.
- An aqueous solution phase is always dominant in the solvent water, that is, H2O. Under specific temperature, pressure and aqueous composition conditions, any other element (such as Fe and C) or substance (such as a pure SO2 gas, stoichiometric phase Cu2S and solution phase (Fe,Ni)1(O,Va)1) have a certain solubility limit in the defined aqueous solution.
- Under certain temperature and pressure conditions, and under given certain concentrations of other dissolved species in the mixture, an O2-dominant gaseous mixture phase can dissolve certain amounts of Fe+2 or Fe+3 species from magnetite (Fe3O4). The magnetite solid has solubility defined relative to the gaseous mixture under the given conditions.
- Under certain temperature and pressure condition, under specific concentrations of other dissolved species in the liquid phase, a Fe-dominant liquid mixture phase can dissolve certain amounts of, for example, Cr and O. The Cr and O components have the solubility defined in the liquid mixture.

Basic Settings and Definitions

In a homogeneous aqueous solution or an aqueous-bearing heterogeneous interaction system, the most essential definition is for system-components there must be `H2O`, `H+1` and `ZE` (electron) plus those for elements dissolved in aqueous solution (such as `Na`, `Cl`, `S`) and associated in interacting metals/alloys (such as `Fe`, `Cr`, `Mn`, `Mg`, `Ni`, `Al`, `Si`, `Zn`). Three fundamental phases in a system are the `AQUEOUS` solution, the `GAS` mixture and the `REF_ELECTRODE`. The `REF_ELECTRODE` phase is used for setting the reference state for electrostatic potential in the system and for calculating the Eh condition (defined as `MUR(ZE)/RNF`). Other phases should be appropriately selected and retrieved from critically-assessed databases that cover not only the target phases (solution or stoichiometric) in interacting metals/alloys but also the secondary phases (solution or stoichiometric). The two public databases PAQ and PAQS are specially designed as single-database choices that cover all kinds of phases necessary for calculations. However, these databases are each limited to a framework of a very small number of elements. When it comes to simulations of complex multicomponent systems with a wide variety of elements and phases, the thermodynamic data must be selected and retrieved from several databases: `AQUEOUS` solution and `REF_ELCTRODE` phases must be retrieved from TCAQ or AQS; alloy phases (such as `FCC_A1`, `BCC_A2`, `HCP_A3`, `CEMENTITE`) from alloy solution databases (such as SSOL for general alloy phases, TCFE for steel/Fe-alloy phases, TCAL for Al-based alloy phases; TCMG for Mg-based alloy phases, and TCNI for Ni-based superalloy phases); gaseous mixture phase and secondary phases from specific substance or solution databases (such as SSUB for `GAS` phase and various solid compound phases or TCOX for oxide solution phases). Note that the `REF_ELECTRODE` phase should always be suspended in equilibrium calculations, while `GAS` phase could be set as `ENTERED`, `SUSPENDED` or `DORMANT`, depending on the purpose of the calculation.

When defining an interaction system, the initial condition for the `H2O` component is always set as 1 kg of water. The initial composition conditions for dissolving and interacting elements are normally defined in moles (such as `n(Fe)=0.009`, `n(Cr)=5E-4`, `n(Ni)=3E-4`, `n(Mn)=5E-5`, `n(S)=5E-5`, `n(Na)=3`, `n(Cl)=3`). This makes it straightforward and convenient to count various related aqueous solution properties based on molality. The initial conditions for the `H+1` and `ZE` components can be given as molar compositions (such as `n(H+1)=0`, `n(ZE)=0`) or their activities or potentials (such as `lnACR(H+1)=-9.21`, `MUR(ZE)=8400`).

The pH and Eh properties of the aqueous solution in the interacting system are always defined in the following way:

```
pH = -log10[ACR(H+1,AQUEOUS)*AH2O]]Eh = MUR(ZE)/RNF
```

The symbol `AH2O` is the molecular weight of solvent H2O (equals `55.508435`) and `RNF` is the Faraday constant (equals `96485.309`).

The activity of the solvent water (`ACRH2O`, `Aw`), the osmatic coefficient of aqueous solution (`OSMC`, `Os`), electronic affinity (`Ah`), electronic activity log10ACRe (`pe`), ionic strength (`IS`), total aqueous concentration, in molality (`TM`) and total alkaline concentrations under two definitions (`At1`/`AT2`) are calculated and listed for each equilibrium state.

POLY3 calculations for mass balances in Thermo-Calc are always based on site-fractions. Consequently, when functions for describing various properties of aqueous solutes are defined, such as molality (`MLi`), activity coefficient (`RCi`) and activity (`AIi`), they should be converted to molality-based quantities:

```
MLi = Y(AQUEOUS,i)*AH2O/YH2O
```

```
RCi = ACR(i,AQUEOUS)*YH2O/Y(AQUEOUS,i)
```

```
AIi = ACR(i,AQUEOUS)*AH2O
```

Here, `YH2O` is the site-fraction of solvent H2O and `AH2O` equals `55.508435`.

Many more variables, functions and tables can be entered for various purposes. For instance, an equilibrium constant for a homogeneous reaction or a solubility product for a solid dissolution reaction can be entered.

Thermodynamic Data Requirements

In this section:

Required Thermodynamic Data

To calculate a Pourbaix diagram, thermodynamic data for at least the following four types of phases must be available:

- The aqueous solution phase which applies a certain aqueous solution model. In Thermo-Calc, information about this phase could be retrieved from, for instance, the TCAQ or AQS database (these also include data for the `REF_ELECTRODE` phase that is used for setting the reference state of the standard hydrogen electrode).
- The alloy solution and/or compound phases for the primary matrix phases (and possibly also for the precipitated phases in the alloy. Examples of such phases include FCC_A1, BCC_A2, HCP_A3, SIGMA and CEMENTITE. In Thermo-Calc, information about such phases could be retrieved from, for example, the TCFE database for steels/Fe-alloys, the TCNI database for Ni-based superalloys, the TCAL database for Al-based alloys, the TCMG database for Mg-based alloys, the TCSLD for Sn-/Au-/Bi-/Zn-based solder alloys or the SSOL for general alloys.
- The secondary solid phases that would form as a result of the heterogeneous chemical or electrochemical reactions. These phases could be, for example, oxides, hydroxides, silicates, hydrous silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates or halides. In Thermo-Calc, information about such phases could be retrieved from, for example, the SSUB database for pure solid compounds or the TCOX database for complex oxide solids.
- The gaseous mixture phase. Information about this phase could be retrieved from, for example, the SSUB database. However, note that is also possible to perform Pourbaix diagram calculations that ignore the gaseous mixture phase.

All this thermodynamic data about the various phases must be critically assessed and internally consistent. Furthermore, when the data is retrieved from several databases, the data taken from each database must be consistent with the data taken from the other databases. When Pourbaix diagrams and other diagrams of steel corrosion processes are calculated, it is typically recommended that the TCAQ, TCFE, SSUB and TCOX databases or the AQS, TCFE, SSUB and TCOX are used in combination.

The public PAQ and PAQS databases each contains thermodynamic data for all four phase types and can be used for calculating Pourbaix diagrams. They have been designed specifically for the purpose of demonstrating the POURBAIX module functionality in Thermo-Calc. However, these databases only allow you to perform test calculations for simple cases with major phases in which only a few elements can be considered.

Including or Excluding the Gas Phase

Under defined pressure and temperature conditions, the solvent water’s thermodynamic stability limits are determined by the following two electrochemical reactions:

```
H2O(water) + 2e- = H2(gas) + 2OH-1
```

```
2H2O(water) = O2(gas) + 4H+1 + 4e-
```

The first reaction describes the formation of H2-dominated gaseous mixture, under reducing conditions. The second reaction describes the formation of O2-dominated gaseous mixture, under oxidising conditions.

If the system reaches global equilibrium, then the water component is electrolyzed to H+ and O-2 at all pH conditions. The degree of electrolysis depends on the pH value in the aqueous solution phase. If Eh gets high enough, then the O-2 anion is oxidized to O2 (aqs). On the other hand, if Eh gets low enough, then the H+ cation is reduced to H2 (aqs). The major electrolysis and redox reactions are the following:

```
H2O (water) = H+ + OH- → Electrolysis of water at all pH.

H2O (water) = 2H+ + O-2 → Electrolysis of water at all pH.

O-2 - 2e- = 0.5O2 (aqs)→Oxidation or de-electronization of O-2 at high Eh.

2H+ + 2e- = H2 (aqs) → Reduction or electronization of H+ at low Eh.
```

At a critically high Eh value under a given pH condition, an aqueous solution phase with a high enough O2 activity becomes less stable than an O2-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system. The replacement process can be characterised by the following phase-transformation on the aqueous-gas phase boundary and oxidation of remaining water:

```
O2 (aqs)  = O2 (gas)

H2O (water) - 2e- = 2H+(gas) + 0.5O2 (gas)
```

Similarly, at a critically low Eh value under a given pH condition, an aqueous solution phase with a high enough H2 activity becomes less stable than a H2-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system, through the following phase-transformation on the aqueous-gas phase boundary and reduction of remaining water:

```
H2 (aqs)  = H2 (gas)

H2O (water) + 2e- = O-2 (gas) + H2 (gas)
```

The phase transformation from an aqueous solution phase to an O2- or H2-dominated gaseous mixture phase also depends on the total molar Gibbs energies of the phases (which are complex functions of the phase constituents, the temperature and the pressure). The Gibbs energy minimization technique used in Thermo-Calc ensures that the phase transformation is accurately simulated.

The following Pourbaix diagrams show the result of a calculation where the gaseous mixture phase was included. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase has been oxidized and reduced, respectively, to an O2- or H2-dominated gaseous mixture phase.

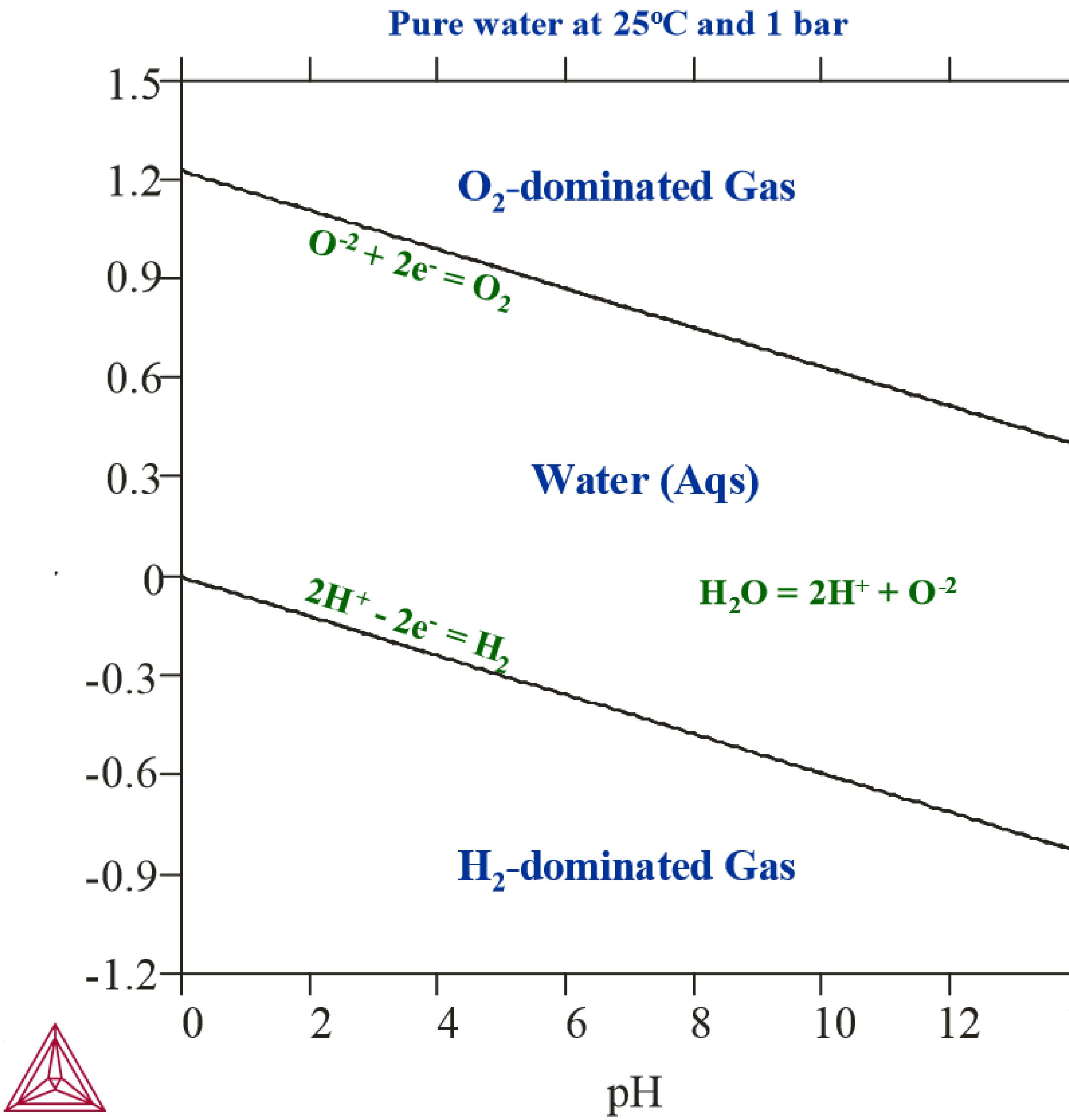
The two example diagrams show that the upper and lower boundaries between the aqueous phase (water) and the gas phase (dominated by either O2 or H2) can shift when solutes dissolve or when the temperature and pressure change.

Accordingly, if one does not take a gaseous mixture phase into account when performing a calculation of Pourbaix diagram (as above), then the aqueous solution phase may end up with an extremely high O2 (aqs) concentration at high Eh condition, or an extremely high H2 (aqs) concentration at low Eh condition. Under either of these two extreme circumstances, the concept of “aqueous solution phase” is no longer valid and consequently no proper aqueous solution model can actually be applied. Therefore, from a restrictive thermodynamic equilibrium point of view, one shall normally include a gaseous mixture phase in an aqueous-bearing heterogeneous interaction system. This is true for all types of equilibrium calculations for an aqueous-bearing heterogeneous interaction system, not only of Pourbaix diagram calculations.

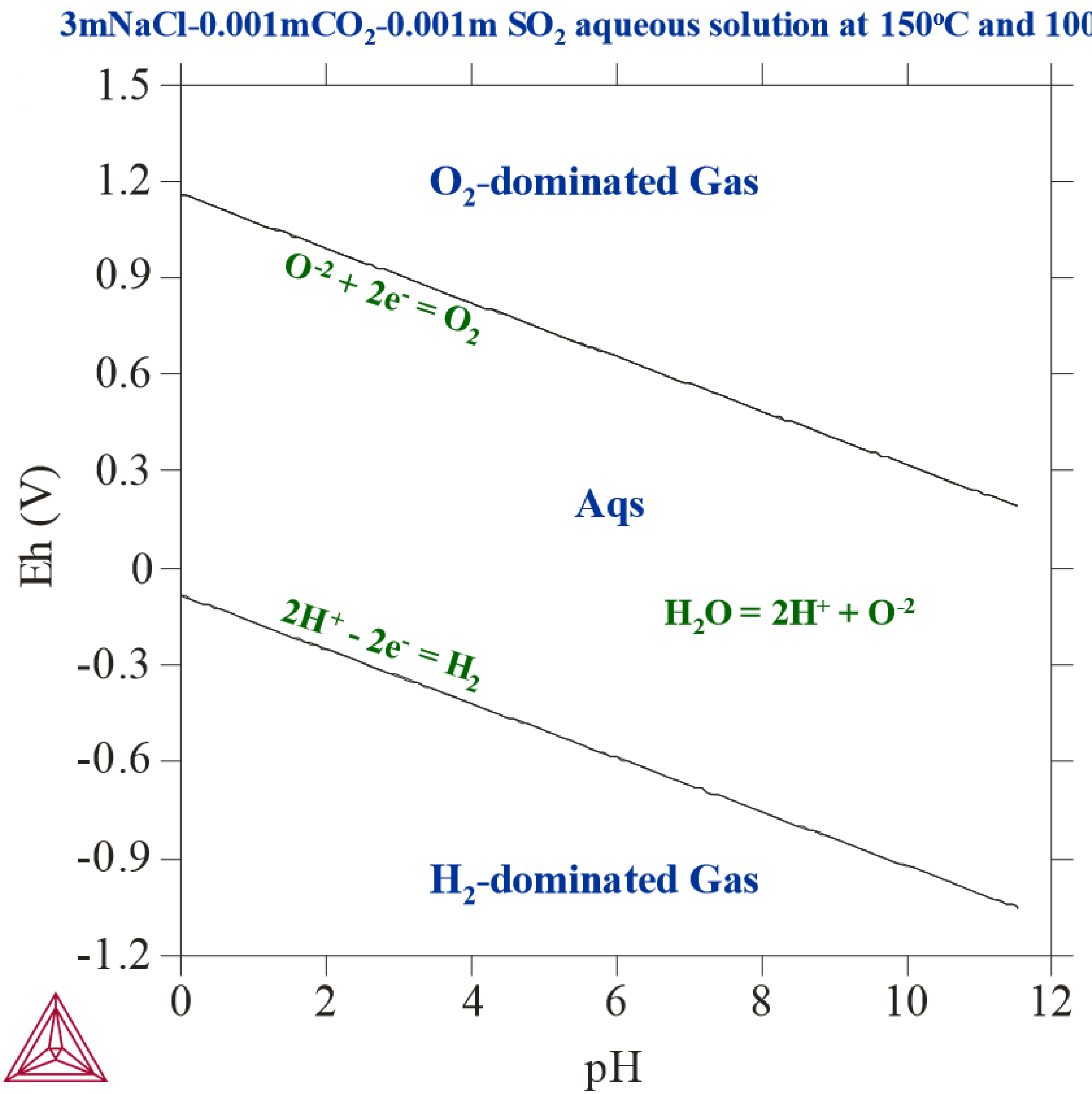
Hence, to perform a completely accurate Pourbaix diagram calculation, the gaseous mixture phase must be taken into account. However, since these electrochemical reactions normally have much higher kinetic barriers and are slower than other electrochemical and chemical reactions in the interaction system, one can sometimes ignore the gaseous mixture phase in the calculation. Note that if the gaseous mixture phase is ignored in this way, then the Pourbaix diagram does not show the H2O-stability limiting lines.

Example Diagrams

The first diagram is a pH-Eh diagram for pure water at 25°C and 1 bar:



The second diagram is a pH-Eh diagram for 3mNaCl-0.001mCO2-0.001mSO2 aqueous solution at 150°C and 100 bar.


3mNaCl-0.001mCO$_2$-0.001m SO$_2$ aqueous solution at 150ºC and 10
O$_2$-dominated Gas
O^{-2} + 2e$^-$ = O$_2$
Aqs
H$_2$O = 2H$^+$ + O^{-2}
2H$^+$ - 2e$^-$ = H$_2$
H$_2$-dominated Gas
Eh (V)
1.5
1.2
0.9
0.6
0.3
0
-0.3
-0.6
-0.9
-1.2
0
2
4
6
8
10
12
pH

Examples of Pourbaix Diagrams for Fe

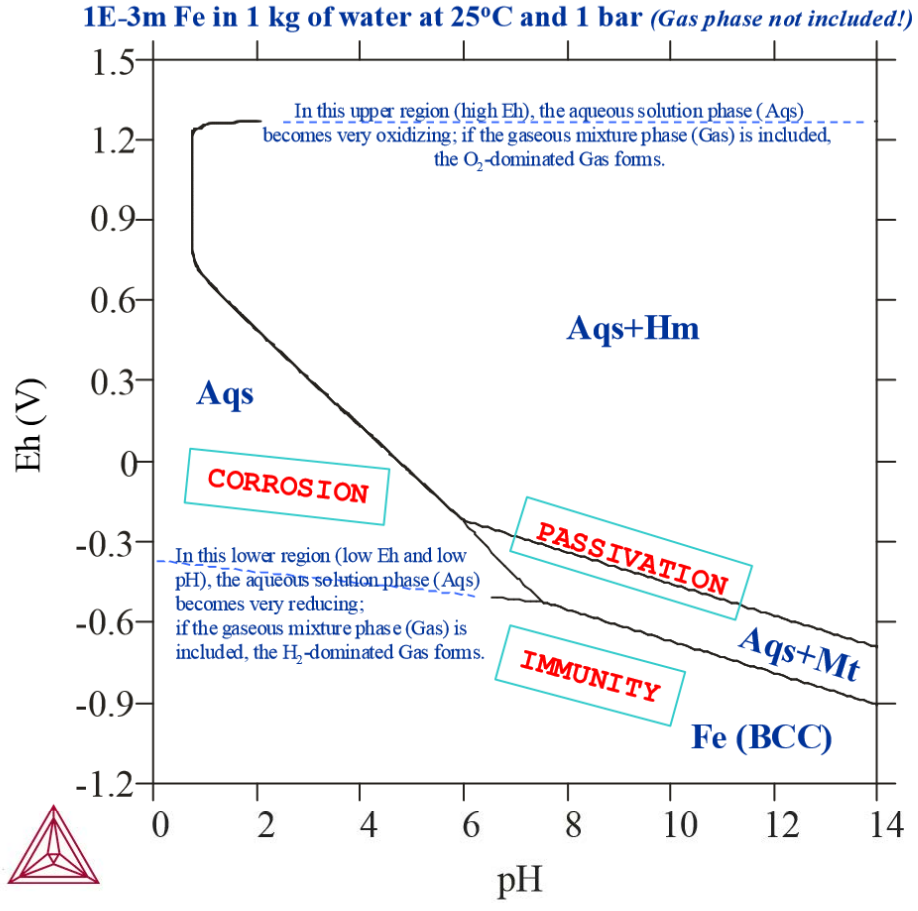
The following two topics are examples of Pourbaix diagrams for Fe. For the first example, the calculations on which the diagrams are based have not taken the gas phase into account. The diagrams in the second example are based on calculations that have taken the gas phase into account.

In this section:

Pourbaix Diagrams with Gas Phase Excluded

This is an example of a Pourbaix diagram of Fe, in which the gas phase has not been considered in the calculation. The system has 0.001 mole of Fe in 1 kg of pure water at a temperature of 25oC and a pressure of 1 bar. Magnetite (Mt, Fe3O4) and hematite (Hm, Fe2O3) co-exist with the Fe-containing dilute aqueous solution. The formation of magnetite and hematite represent the passivation of iron in the upper right pH-Eh field.

If pH is low and Eh is relatively high, then Fe eventually completely dissolves into the aqueous solution phase. Under conditions of low Eh, Fe remains in its stable solid state, the BCC phase, and neither dissolves into water nor into alternates to Fe (the immunity of Fe).

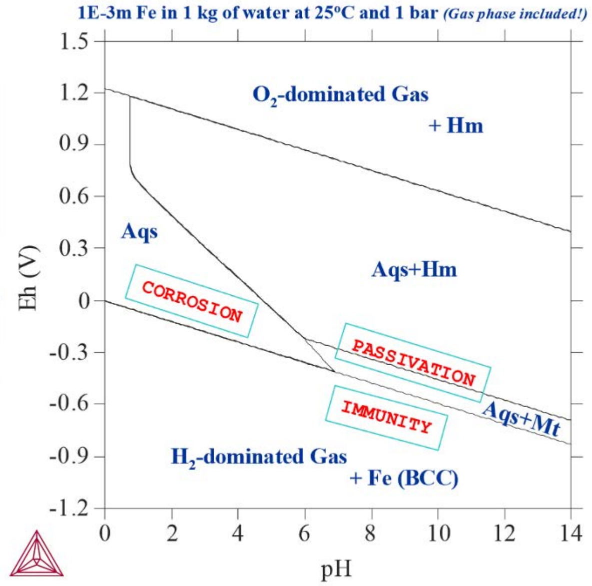


In this upper region (high Eh), the aqueous solution phase (Aqs) becomes very oxidizing; if the gaseous mixture phase (Gas) is included, the O_2-dominated Gas forms.

In this lower region (low Eh and low pH), the aqueous solution phase (Aqs) becomes very reducing; if the gaseous mixture phase (Gas) is included, the H_2-dominated Gas forms.

Pourbaix Diagrams with Gas Phase Included

With all the possible redox reactions involving the aqueous solution phase and gaseous mixture phase being considered in the equilibrium system, that is, the gaseous mixture phase is included in the calculation, the Pourbaix diagram of Fe in a system with 0.001 mole of Fe in 1 kg of pure water at 25oC and 1 bar.



Comparing this Pourbaix diagram with that from *Basic Settings and Definitions* on page 7, you can see that both diagrams are for the same interaction system under the same temperature-pressure condition, but the present diagram shows the results of calculations where the gaseous mixture phase has been included. It presents the complete Pourbaix diagram for the defined interaction system, in a full thermodynamic equilibrium. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase is oxidised and reduced to the O2- or H2-dominated gas phase. Hematite coexists with the O2-dominated gas, while Fe-BCC is stable with the H2-dominated gas. The stability field of magnetite may extend slightly into the H2-dominated gas region, where it coexists with the gaseous mixture instead of the aqueous solution. Its boundary with Fe (BCC) cannot be drawn due to the absence of aqueous solution phase.

It is not possible to calculate the pH value in both the O2- and H2-dominated gaseous mixture phase stability regions where the aqueous solution phase is absent. Hence, in a normal Pourbaix diagram, no line is drawn that indicates a phase boundary between the gas phase and the metallic phases or secondary phases (that is, metal-oxides).

Other Examples of Pourbaix Diagrams

In this section:

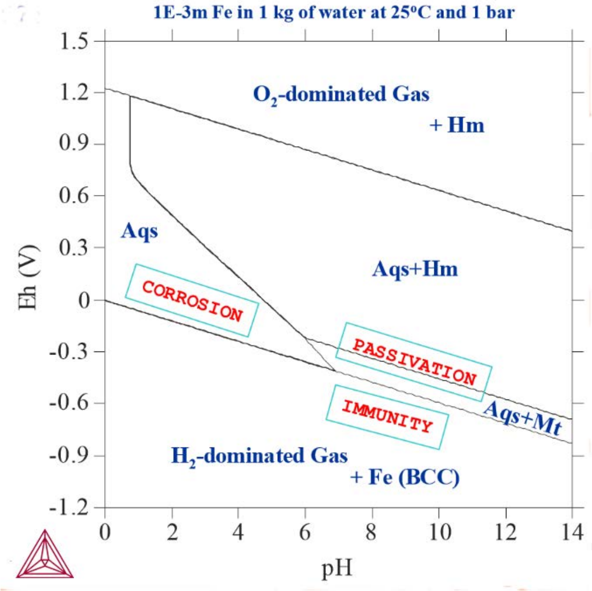
Variations of Pourbaix Diagrams

The shape of a Pourbaix diagram of an alloy or condensed material and the stability relations of various secondary phases depend upon the following system factors:

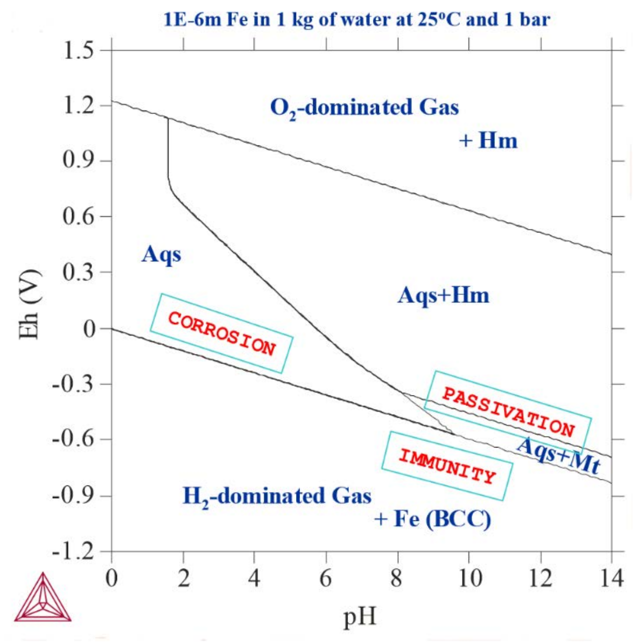
- Initial amount of the alloy or other condensed materials
- Initial composition of the alloy or other condensed materials
- Initial amount of the interacting aqueous solution phase
- Initial composition of the interacting aqueous solution phase
- Temperature and pressure conditions

In the interaction system that the diagrams in *Pourbaix Diagrams with Gas Phase Excluded* on page 16 and *Pourbaix Diagrams with Gas Phase Included* on page 16 are based on, the initial amount of pure Fe that was taken to have effectively reacted with 1 kg of pure water at 25°C and 1 bar was 0.001 m. The following diagrams are Pourbaix diagrams of Fe where other initial amounts of pure Fe have been used, or where the interacting aqueous solution compositions have been alternated, or the temperature and/or pressure have been changed. Gaseous mixture phases have been included in all the calculations that these diagrams are based on.

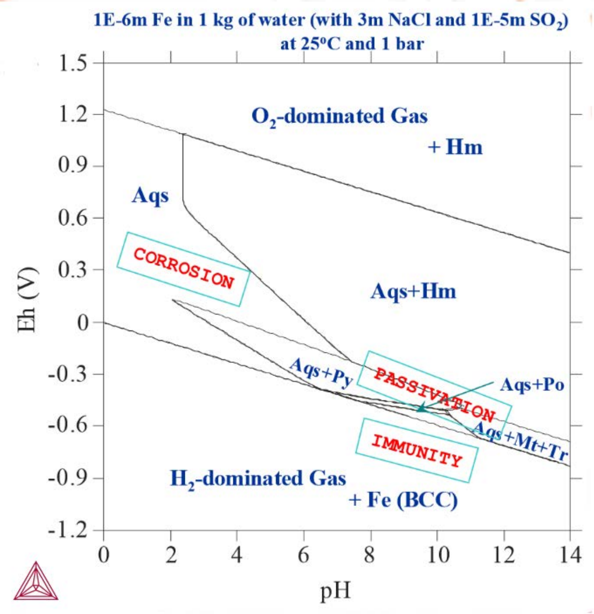
In the first diagram, 1E-3 m Fe actively reacted with 1 kg of pure water at 25°C and 1 bar (as in the calculation in Pourbaix Diagrams with Gas Phase Included):



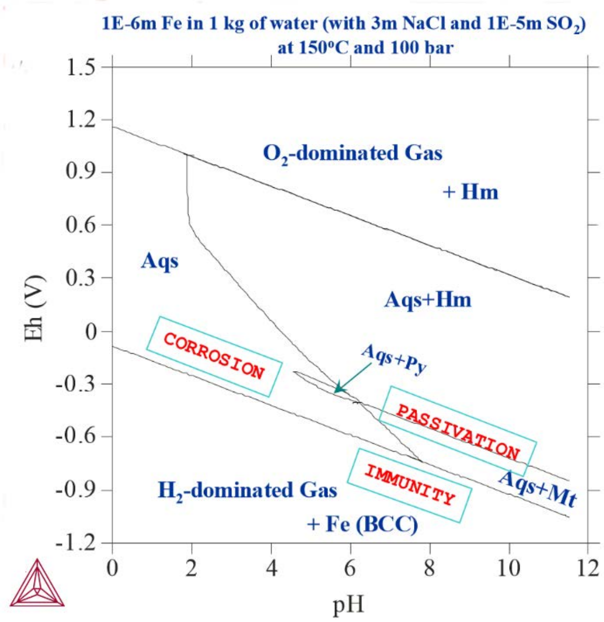
In the second diagram, 1E-6 m Fe actively reacted with 1 kg of pure water at 25°C and 1 bar. Note that the active metal corrosion region gets enlarged as the initial Fe amount decreases from 1E-3m to 1E-6m:



In the third diagram, 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO2 at 25°C and 1 bar. Introducing SO2 into the system leads to the formation of various metal-sulphides (Py-pyrite, Popyrrhotite, Tr-troilite). In addition, the passivation region becomes larger.



Finally, in the fourth diagram, 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO2 at 150°C and 100 bar. Here, changing the temperature and pressure affects the stability fields of various Fe-oxides/sulphides.

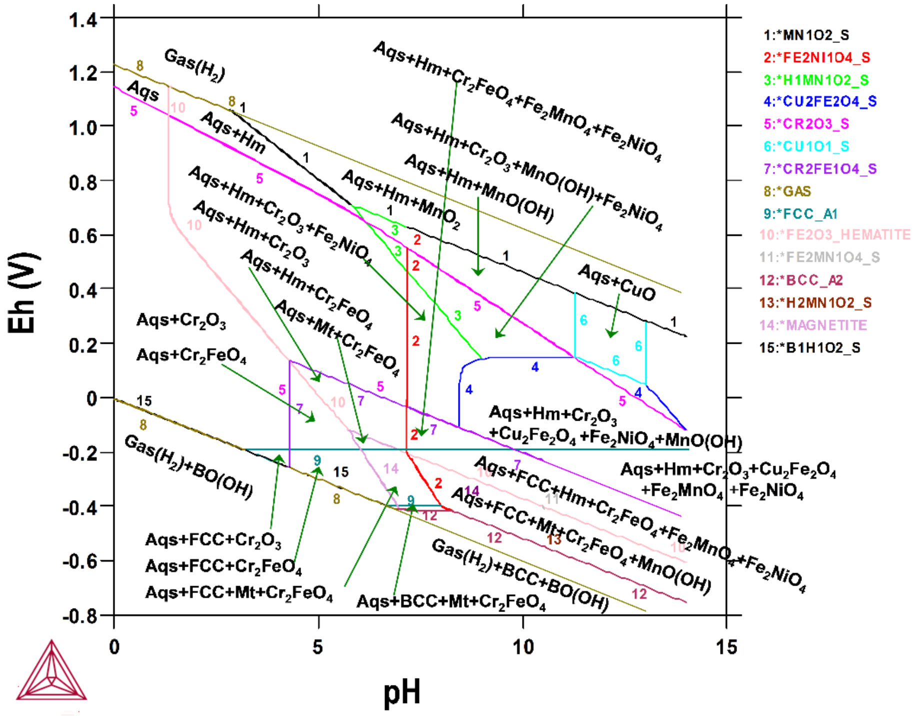


As you can see from the four diagrams, the aqueous-gas phase boundaries shift as the initial bulk compositions, pressure and temperature conditions in the interaction system change.

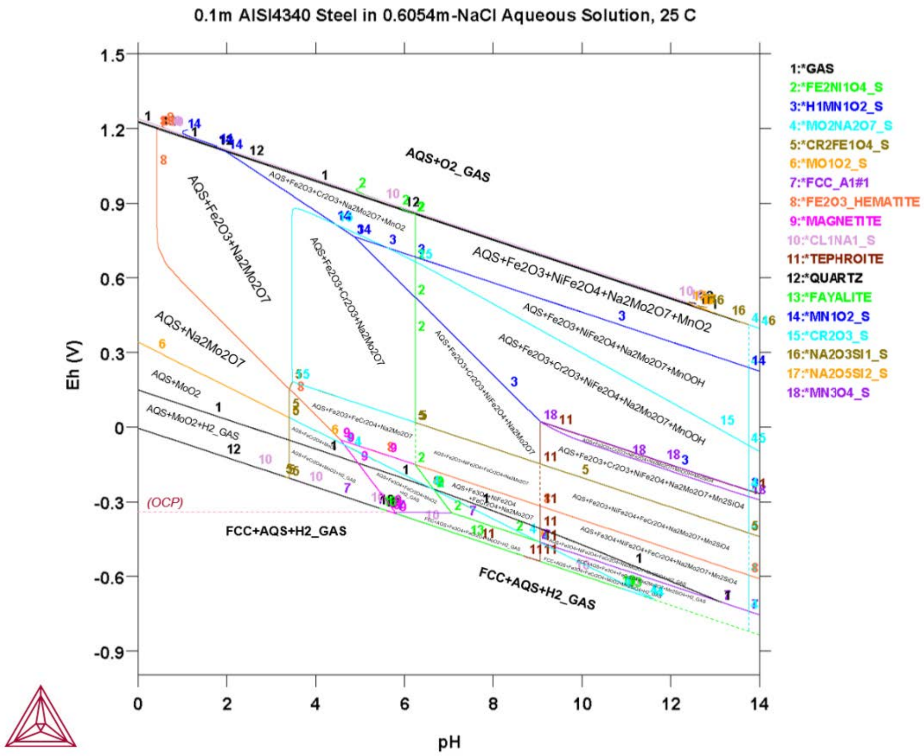
Pourbaix Diagrams for Complex Alloys

Thermo-Calc can not only be used to simulate how pure metals interact with pure water or simple aqueous solutions under normal pressure and temperature conditions. It can also be used to calculate how complex alloys and concentrated aqueous solutions interact over a very wide pressure, temperature and composition ranges. This is illustrated with the two examples.

The first example is a Pourbaix diagram calculated for the heterogeneous interaction between 0.001 mole of steel (Fe-7.676Cr-5.0Ni-2.1887Mn-1.0Cu [at%]) and 1 kg of water (and with 1.2 m H3BO3, 0.022 m Li and 0.001 m NH3), at 25°C and 1 bar. This application is particularly useful for safety assessments of nuclear reactors and nuclear waste repositories.



The next example is a Pourbaix diagram calculated for the heterogeneous interaction systems between 0.1 mole of AISI4340 stainless steel (Fe-0.80Cr-1.85Ni-0.70Mn-0.25Mo-0.25Si-0.40C [wt%]) and 1 kg of seawater (with the equivalent of 0.6054 m NaCl), at 25°C and 1 bar. This application is particularly useful for failure analysis of petroleum exploitation industry.



Pourbaix Diagram References

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DATAPLOT User Guide

Thermo-Calc Version 2016b

Introduction to the DATAPLOT User Guide

In this section:

Using this Guide

The *DATAPLOT User Guide* gives all the details on the graphical language DATAPLOT that a phase diagram or property diagram calculated by Thermo-Calc or a kinetic profile simulated by the Diffusion Module (DICTRA) can be defined.

This guide

- Discusses the important features of the DATAPLOT language.
- Describes the commands to define PROLOGUE and DATASET.
- Several examples and the standard codes for formatting are provided.

A topic introduce the method of formatting DIGLIB symbols in LaTeX documents, for the purpose of necessarily/appropriately referring to the corresponding LaTeX symbols (closest to those DIGLIB symbols which have been plotted on a diagram using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

About the DATAPLOT Graphical Language

In order to obtain graphical output of any numerical data and informative strings, a graphical language called DATAPLOT was developed in connection with the graphical software DIGLIB. Using this graphical language, you can store information in a normal text file (*.EXP), which can be plotted as graphical symbols, lines, texts or Greek letters on any plot device support by DIGLIB.

You can generate and plot DATAPLOT (*.EXP) files together with various calculation and/or experimental results from, for example, phase and property diagrams calculated with the Thermo-Calc software composition profiles or other diagrams simulated by the Diffusion Module (DICTRA).

An EXP file automatically generated by the POST-processor (using the *MAKE_EXPERIMENTAL_DATAFILE* on page 199 command) in the Thermo-Calc software is a DATAPLOT (*.EXP) file and may contain all types of legal DATAPLOT commands and parameters. With a text editor, you can modify or add some DATAPLOT commands and related parameters in an existing EXP file. This is useful when appending experimental information to calculated/simulated plots, and when specifying user-defined texts, symbols, colors, fonts, filled patterns, diagram types, diagram sizes, symbol/character sizes, titles, special characters, etc.

DATAPLOT Examples

To help you prepare your EXP (experimental) files to use for your plotted diagrams generated by Thermo-Calc simulations, there are examples of EXP files using the DATAPLOT graphical language standard, which are normally independent of software versions.

Using DATAPLOT Graphical Language

In this section:

DATAPLOT File Structure

A DATAPLOT file is a normal text file with the extension `EXP` that can be created with a text editor or by a program. The file must contain one or more `DATASETS` and possibly also one or more `PROLOGUES`. Each `PROLOGUE/DATASET` is an entity that can be individually selected for plotting.

A PROLOGUE/DATASET is identified by a unique positive number in the file. A PROLOGUE normally contains various DATASET commands for defining information about axis scaling, axis text, axis length, title and so on. A PROLOGUE is terminated by another PROLOGUE or by the first DATASET. This means that all PROLOGUES must be placed at the beginning of the file, before the first DATASET.

A DATASET normally contains DATASET commands that are associated to separate data points, as well as with one or more `BLOCKS` of data (calculated or experimental). A DATASET is terminated by another DATASET command or the end of file.

DATAPLOT Language Syntax

The DATAPLOT language consists of commands with or without parameters:

```
COMMAND {parameter(s)}
```

The basic graphical command consists of an X/Y coordinate pair and a Graphical Operation Code (`GOC`). With other commands, the interpretation of this basic command can be modified. There are separate commands to draw a polygon or a function and ways to get texts in different fonts.

To edit a DATAPLOT file, the graphical commands can be abbreviated.

A command (with parameters) must not exceed 80 characters. If it is too long (normally as writing necessary codes in a command’s parameters for a complex expression), two or more lines can be edited.

Coordinate Systems

The DATAPLOT language accepts coordinates in three different coordinate systems, which are called *word*, *virtual* and *normalized*.

- The *word* coordinates are selected to represent any kind of data and be of “any” magnitude.
- The *virtual* coordinate system uses centimeters as units. However, the actual size of one unit is dependent on the implementation of the device driver in DIGLIB. It is not recommended to use this coordinate system if different output devices are used for preliminary and final plots.
- The *normalized* coordinate system goes from zero to one. When plotting, you interactively scale each axis by selecting the minimum and maximum word coordinates on the axis. In the normalized coordinate system, the minimum axis value is represented by

zero and the maximum by one. DIGLIB draws a square between the four points (of the X and Y axes) that are determined by the coordinates zero and one in the normalized coordinates.

It is also possible to draw triangular plots as described below. However, in most places, it only references square diagrams. All data points within the minimum and maximum word coordinates are plotted inside this square. DIGLIB also writes tic marks and corresponding word values at such tic marks.

It may be convenient to use normalized coordinates to draw boxes and texts. You can give normalized coordinates outside zero and one if you want to write texts outside the area enclosed by the square. To ensure proper operation outside the normalized box, the clipping must be turned off.

Graphical Operation Codes

The Graphical Operation Code (`GOC`) determines how the coordinates are interpreted and what is done at the point determined by the coordinates. For an individual data point, its GOC codes must be given. For each data *BLOCK* on page 19, you define a default GOC that is used for the whole BLOCK, unless a GOC is explicitly defined for a specific point.

- If `S` is omitted, no symbol is plotted. A number selecting the symbol can optionally follow the character `S`. The DIGLIB software determines which symbol the number represents. See *Plotting a Symbol* on page 9.
- If any of the other characters are omitted, the default defined for the BLOCK is used. Absolute values imply the current coordinates; relative values mean that these are added to the current coordinates. The GOC must be written without any space between various characters, but the order for the characters is irrelevant.
- If no `GOC` is defined for a BLOCK, the system default is `MWA`, (Move Word Absolute), i.e., move to the given point that is interpreted as absolute word coordinates. `GOC=DNA` means draw a line from the current point to the new one interpreting the coordinates as normalized. After each draw or move operation, the so-called current point is the new point.
- The *TEXT* on page 27 following the `'` command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or *STRING* on page 25 names using the ~ descriptor. To get PostScript outputs, the TEXT must be edited by the LaTeX Text Formatting Program instead (see *LaTeX Formatting Codes* on page 12).

GOC Character Definitions

The GOC is a combination of the following characters:

Character	Meaning
`W`, `V` or `N`	To use word (`W`), virtual (`V`) or normalized (`N`) coordinates. `W` is the default.
`A` or `R`	XY are absolute (A) or relative (R) values. `A` is the default.
`M` or `D`	To perform a move (M) or draw (D) operation to XY. `M` is the default.
`B`	To apply “soft” splines on a line drawn between the coordinate pairs (used only on BLOCK data).
`S`	To plot default symbol at XY.
`S#`	To change default symbol to No # symbol and plot it at XY.
`'TEXT`	To plot `TEXT` at XY. It must be the last operation in a GOC code. The TEXT following the ’ command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor.

Tables or Blocks

In many cases, you have (calculated or experimental) data in the form of tables, and want to plot one or several columns as X-axis and one or more columns as Y-axis. A single table can contain many sets of data records of the same kind of information for a specific data *BLOCK* on page 19. There can be many data BLOCKS in a *DATASET* on page 19.

By enclosing these tables in a data BLOCK, you can select which column(s) is the X-axis and which is the Y-axis. For example,

```
BLOCK X=C1; Y1=C3; Y2=C2; GOC=C4,DAW
```

Where the X-axis values are in column 1, the Y-axis values are in columns 2 and 3, and any GOC codes are in column 4. The default GOC for this BLOCK is Draw Absolute Word. The GOC code inside the table is only necessary if the default GOC is not applicable.

A more elaborate use of the table is shown in this example:

```
BLOCK X=C3; Y=1E3/(C3+273); GOC=C8,MAWS1
```

Where the X-axis values are in column 3, the Y-axis values are in column 1 with some additional calculations applied. Any GOC is in column 8, and the default GOC is Move Absolute Word and plot the symbol no. 1.

Columns in a table must be separated by one or more space characters and do not have to be justified.

It is possible to have tables with mixed text and numbers, but each word followed by a space is counted as one column. The columns used for plotting also must be numerical. An example of a legal line in a table is

```
298.15 This_is_the_second_column 11.5 This_is_the_fourth_column
```

> A line in the table must not exceed 80 characters. A BLOCK must be terminated by a line with the *BLOCKEND* on page 20 command.

Drawing a Polygon

Normally, each point is written on a separate line. But in order to draw a line in a more compact way, use the command *DRAWLINE* on page 21. DRAWLINE is followed by a couple of X/Y number pairs. The X/Y pairs must be separated by a space, and there must be a comma sign between the X and Y values. DRAWLINE makes a move operation to the first pair of X/Y coordinates, and then draws a line among all pairs up to the last one. All pairs must fit on one line of 80 characters, but there can be several consequent DRAWLINE commands.

Drawing an Analytical Function

Use a *BLOCK* on page 19 command to set an axis to a function. It is not necessary to use a value from any column in order to compute the function value to be plotted. Use the *FUNCTION* on page 27 command to plot a function with an even increment of the independent variable.

Painting of an Enclosed Area

Use the *PAINT* on page 27 command to paint or fill an area in a specified pattern in the plot. Available patterns are determined by the DIGLIB software. A related command to PAINT is *PCFUNCTION* on page 27.

Writing a Text

Use the *TEXT* on page 27 command to write a text at the current point. You can write a text at any X/Y pair by appending a single quote followed by the text on the same line. For example:

```
1.1 1.0 NAM'This is a text
```

writes `This is a text` at the normalized coordinates (`1.1, 1.0`).

Use the command *FONT* on page 24 to select the font used for the text, and *CHARSIZE* on page 22 to select the size of the characters. Set this size of the symbols with *SYMBOLSIZE* on page 22.

If a text or a single character should be of a different font than all the other text, or to use subscripts or superscripts in a text, use the ^ operators or STRING command to create the text. The command *STRING* on page 25 stores the text in a specified variable that includes all text-formatting information defined by the DIGLIB software. See *Example 3 – Using Strings and Various Line Types* on page 32 and *Example 5 – Use Included Files for Predefined Symbols* on page 34.

However, if a graphical output is done on a PostScript device using the PostScript hardcopy fonts, special text formatting codes as *LaTeX Formatting Codes* on page 12 should be used and the STRING formatting syntax is then not valid.

Plotting a Symbol

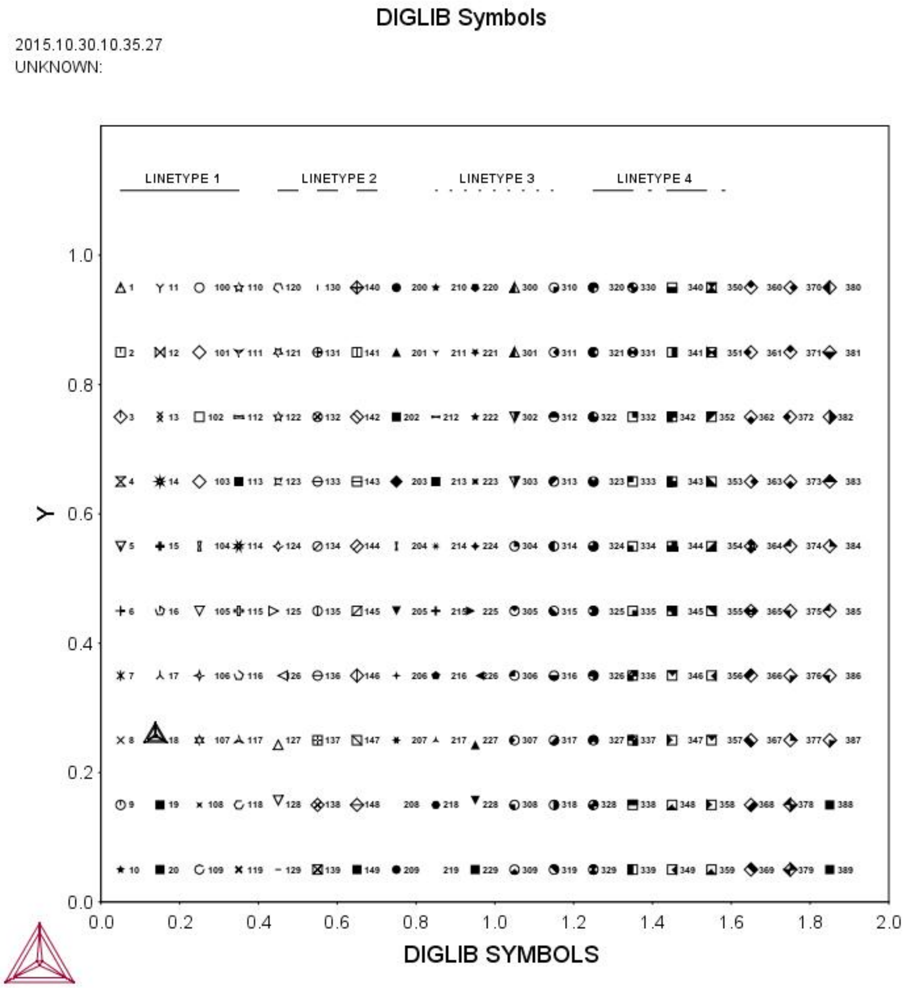
As described in *Graphical Operation Codes* on page 6, a GOC code in a data BLOCK may contain an `S` option to plot a symbol for an X/Y pair or the same symbols for the data BLOCK. A number selecting the symbol can optionally follow the character `S`. You can plot a symbol at any current X/Y position by appending a quote specified by the symbol number in the GOC code (e.g., `1.1 1.0 MANS5'This is a text`).

You can also insert DIGLIB symbols into LaTeX-edited documents.

DIGLIB symbols available in Thermo-Calc

The image summarizes all the standard symbols available in the DIGLIB software. A default symbol is the current symbol in the run of the software (it is usually the No 1 symbol if the POST-processor is switched on for the first time). S (i.e., # is not specified) means that the current symbol is plotted. S0 (i.e., #=0) means that no symbol is plotted.

All the DIGLIB symbols work properly and give good output results for the PostScript format.



Other Commands

Use the *LINETYPE* on page 21 command to define line types as solid, long dashed, short dashed or dotted. If you are using a color device, use the *COLOR* on page 22 command to change color of the lines. On some black and white devices, colors are simulated with different width and dashing of the lines.

- Use the *CLIP* on page 20 command to change the default where all data outside the normalized coordinates zero and one are not plotted.
- When plotting symbols representing various experimental data, it is important that the symbols are centered around the coordinate values.
- Use the *ATTRIBUTE* on page 20 command to change the coordinates where text is displayed. The default is the lower left corner of the first character in the text.
- Use the *INCLUDE* on page 28 command to create libraries with texts and include these in similar plots.

- The dollar sign $ as the first character of a line stands for a comment character, which means the whole line is ignored when plotting.

Interactive Plotting

The DATAPLOT file is read into the POST module in the workspace with *APPEND_EXPERIMENTAL_DATA* on page 192 or *QUICK_EXPERIMENTAL_PLOT* on page 201. These commands ask for the name of the DATAPLOT file and also which PROLOGUE(S) and DATASET(S) are to be plotted.

See the *Thermo-Calc Command Mode Reference Guide* for details about these commands.

By giving the PROLOGUE/DATASET number as `-1`, you get a list of the available PROLOGUES/DATASETS in the file. Note that if `DATASET 0` is in a DATAPLOT file, its data is always used even if other DATASETS are chosen.

Formatting DIGLAB Symbols in LaTeX Documents

When using the LaTeX editor, you can use the DIGLIB symbols in texts and in figures. This then refers to the corresponding LaTeX symbols (closest to those DIGLIB symbols which are plotted on a plot using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

This topic shows how to generate some DIGLIB symbols in texts, through the attached LaTeX source file and its converted jpg file.

DIGLIB_Sym.tex

```
\documentclass[dvips,12pt]{article}

\textwidth 165mm

\textheight 225mm

\oddsidemargin 1mm

\evensidemargin 1mm

\topmargin 1mm

%%\usepackage{amssymb}

%% next replace amssymb and to get udtimes

\usepackage[utopia]{mathdesign}

\usepackage{rotating}

\usepackage[latin1]{inputenc}

\usepackage{graphics}

\usepackage{graphicx,subfigure}% with figures

%\usepackage[draft]{graphicx}% without figures

\usepackage{subfigure}% with figures

\topmargin 1mm

\oddsidemargin 1mm
```

```
\evensidemargin 1mm
\begin{document}
{\Large \bf Diglib symbols and their corresponding LaTeX symbols}
\vspace{5mm}
```

The information below gives the closest corresponding LaTeX symbol. All symbols (except +) must be generated in math mode. Most of these require the package `amssymb`, i.e., you need a directive `usepackage{amssymb}` in the preamble. Two of the symbols require the more extensive `mathdesign` that can be included with `usepackage[utopia]{mathdesign}`.

```
\vspace{5mm}
{\Large
\begin{tabular}{llll}
Diglib & Latex & Latex name & Note\\
1& $\vartriangle$& $\backslash$vartriangle & amssymb \\
2& $\square$& $\backslash$square\\
3& {\Huge $\diamond$} & $\backslash$diamond & size $\backslash$Large \\
4& $\udtimes$& $\backslash$udtimes & mathdesign \\
5& $\triangledown$& $\backslash$triangledown & amssymb\\ 6 & +& normal + \\
7& $\ast$& $\backslash$ast & amssymb\\
8& $\times$& $\backslash$times \\
9& {\Huge $\circ$}& $\backslash$circ & size $\backslash$Large \\
10& {\Huge $\star$}& $\backslash$star & size $\backslash$Large, amssymb\\
11& $\curlyvee$& $\backslash$curlyvee & amssymb\\
12& $\Join$& $\backslash$Join\\
13&& - & nothing similar, overlapping $> <$\\
14&& - & nothing similar, 10-edged star \\
15& $\maltese$& $\backslash$maltese& mathdesign \\
16&& - & nothing similar, a pentagon \\
17& $\curlywedge$& $\backslash$curlywedge & amssymb\\
\end{tabular}}
\end{document}
```

LaTeX Formatting Codes

For a list of supported LaTeX commands, see: http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html

By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.

As of Thermo-Calc 2015a the LTEXT text formatting is replaced by LaTeX. For existing users who may have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent:

LTEXT vs LaTeX Commands for Labels

Symbol or text format	**LTEXT**	**LaTeX**
Subscripts in an axis text	S-A-TEXT Y N Mole-fraction Al^DO2O^DO3	S-A-TEXT Y N \latex Mole-fraction Al_2O_3
Label with subscript	add .13 .15 n c-ZrO^DO2$	add .13 .15 n \latex c-ZrO_2
Greek symbol	ADD .05 .50 N ^GRd$	ADD .05 .50 N \latex \delta

PROLOGUE Commands

In this section:

PROLOGUE

PROLOGUE is the beginning of a number of consequent lines of user-defined diagram layout commands. The lines are displayed with the `optional text` when using the `-1` option in the POST-processor as prompted for the PROLOGUE number with *APPEND_EXPERIMENTAL_DATA* on page 192 or *QUICK_EXPERIMENTAL_PLOT* on page 201.

Syntax	`PROLOGUE # optional text`
	`#` is an unsigned integer identifying the PROLOGUE.

XSCALE

XSCALE sets the scaling in word coordinates of the X-axis.

Syntax	`XSCALE min max`
	`min` and `max` are real numbers.

YSCALE

YSCALE sets the scaling in word coordinates of the Y-axis.

Syntax	`YSCALE min max`
	`min` and `max` are real numbers.

XTEXT

XTEXT sets the X-axis text.

Syntax	`XTEXT text`
	`text` is an arbitrary text string that may contain text-formatting codes.

YTEXT

YTEXT sets the Y-axis text.

Syntax	`Y TEXT text`
	`text` is an arbitrary text string that may contain text-formatting codes.

XTYPE

XTYPE sets the X-axis type as linear (default), logarithmic or inverse.

Syntax	`XTYPE type`
	`type` is a character string reading LIN, LOG or INV.

YTYPE

YTYPE sets the Y-axis type as linear (default), logarithmic or inverse.

Syntax	`Y TYPE type`
	`type` is a character string reading LIN, LOG or INV.

XLENGTH

XLENGTH sets the X-axis length to approximately # centimeters.

Syntax	`XLENGTH #`
	`#` is a positive real number (the approximate X-axis length in centimeters).

YLENGTH

YLENGTH sets the Y-axis length to approximately # centimeters.

Syntax	`Y LENGTH #`
	`#` is a positive real number (the approximate Y-axis length in centimeters).

TIC_TYPE

TIC_TYPE sets the relative length of the tic marks.

Syntax	`TIC_TYPE #`
	`#` is a real number. Default value is 1. Negative number gives tics on the inside of the diagram frame. 0 gives no tics.

TITLE

TITLE sets the title text string to be printed above the diagram.

Syntax	`TITLE text`
	`text` is an arbitrary text string that may contain text-formatting codes

DIAGRAM_TYPE

DIAGRAM_TYPE sets the diagram type to square (the default) or triangular.

Syntax	`DIAGRAM_TYPE type plot_3rd_axis clip_along_third-axis`
	`type` is a character string reading SQUARE (default) or TRIANGULAR. If `type` reads TRIANGULAR, then two additional parameters are given: `plot_3rd_axis` and `clip_along_third-axis` that are characters strings reading YES or NO.

DATASET Commands

In this section:

DATASET

DATASET indicates the beginning of a number of consequent lines comprising a set of user-defined data. The DATASET lines are displayed on the terminal along with the `optional text` when using the `-1` option in the POST-processor as prompted for the DATASET number in the *APPEND_EXPERIMENTAL_ DATA* on page 192 or *QUICK_EXPERIMENTAL_PLOT* on page 201 command.

Syntax	`DATASET # optional text`
	`#` is an unsigned integer identifying this set of data.

BLOCK

BLOCK defines how the following numeric data block shall be interpreted. The definitions of X and Y coordinates may also be expressed as a function of the column values, making it possible to perform transformations.

Syntax	`BLOCK X&=C#; ...; Y&=C#; ...; GOC=C#,@@@...`
	`&'` are optional unsigned integers that make it possible to plot several (maximum 9) X- or Y- axis columns. `#'` are unsigned integers identifying the column numbers. The column number # in "GOC=C#" is the location of any possible GOC codes in the current data BLOCK; @@@ stands for the default Graphical Operation Code (GOC) for the current BLOCK. The GOC code inside the current table is only necessary if the current default GOC is not applicable.

GOC Characters

The GOC is a combination of the following characters:

Character	**Meaning**
`W`, `V` or `N`	To use word (`W`), virtual (`V`) or normalized (`N`) coordinates. `W` is the default.
`A` or `R`	XY are absolute (A) or relative (R) values. `A` is the default.
`M` or `D`	To perform a move (M) or draw (D) operation to XY. `M` is the default.
`B`	To apply "soft" splines on a line drawn between the coordinate pairs (used only on BLOCK data).
`S`	To plot default symbol at XY.
`S#`	To change default symbol to No # symbol and plot it at XY.

Character	Meaning
`'TEXT`	To plot `TEXT` at XY. It must be the last operation in a GOC code. The TEXT following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor.

BLOCKEND

Syntax	BLOCKEND
	BLOCKEND terminates the local definition of the graphical operation code defined by the earlier BLOCK command.

DATAPOINT

DATAPOINT is not a DATASET command, but the basic DATAPLOT command (see synopsis below) performs an action at the current point determined by the specified X/Y- coordinates. A DATASET may contain various data points, in addition to one or more data *BLOCK* on the previous pages. Such data points are separated and independent on each other.

Syntax	`X Y GOC`
	X and Y are unsigned real numbers identifying the X/Y-coordinates for the current data point. GOC stands for Graphical Operation Code (GOC) for the current point. Legal GOC characters. **Example**

```
0.7 0.95 N'Example 6
0.5 0.08 MNA'E^FS18^SQ(^SK^FS10A+5#8*C#^FS10
-!a^FS18)^FS11+B^DIa#b#$
```

CLIP

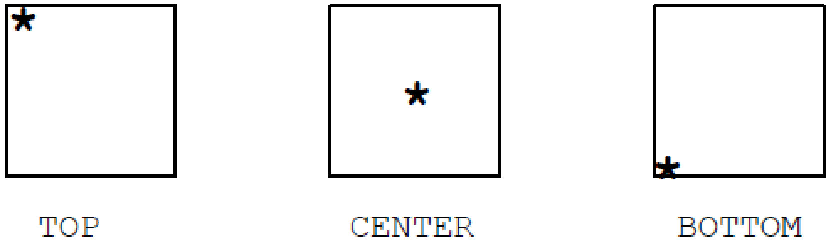
CLIP turns clipping on or off. If it is OFF, it allows output outside the ordinary plot area defined by normalized coordinates zero and one.

Syntax	`CLIP CLP`
	`clp` is a character string reading ON or OFF.

ATTRIBUTE

ATTRIBUTE specifies where the current XY position is in the character or symbol plotbox.

Syntax	ATTRIBUTE
Prompts	`attribute`
	`attribute` may be TOP, CENTER or BOTTOM. ATTRIBUTE CENTER is default for symbols; ATTRIBUTE BOTTOM is default for characters.



LINETYPE

LINETYPE redefines the current linetype in the plot.

Syntax	`LINETYPE #`
	`#` must be an unsigned integer. Legal linetypes are (for both normal graphical outputs and for PostScript formats): • Solid (default) • Long dashed • Short dashed • Dotted

DRAWLINE

DRAWLINE draws a line starting at (x1,y1) to (xn,yn) through (x2,y2) → (x(n-1), y(n-1)).

Syntax	`DRAWLINE x1,y1 x2,y2 .... xn,yn`
	`x` and `y` may be reals or integers of any value. This is the same as connecting all points in a table:

```
x1   y1    M
x2   y2    D
...  ...   D
xn   yn    D
```

CHARSIZE

CHARSIZE redefines the default size of the characters in the plot. The character size has an initial default value, which may vary with the current font setting and the output device (the plot format).

Syntax	`CHARSIZE $$`
	`$$` must be an unsigned real.

SYMBOLSIZE

SYMBOLSIZE redefines the current symbol size setting. The symbol size has an initial default value.

Syntax	`SYMBOLSIZE $$`
	`$$` must be an unsigned real.

GLOBALSIZE

GLOBALSIZE redefines the default global size of the plot. The global size has an initial default value.

Syntax	`GLOBALSIZE $$`
	`$$` must be an unsigned real.

COLOR

COLOR redefines the current color setting. There are 22 legal color codes (from 0 to 21).

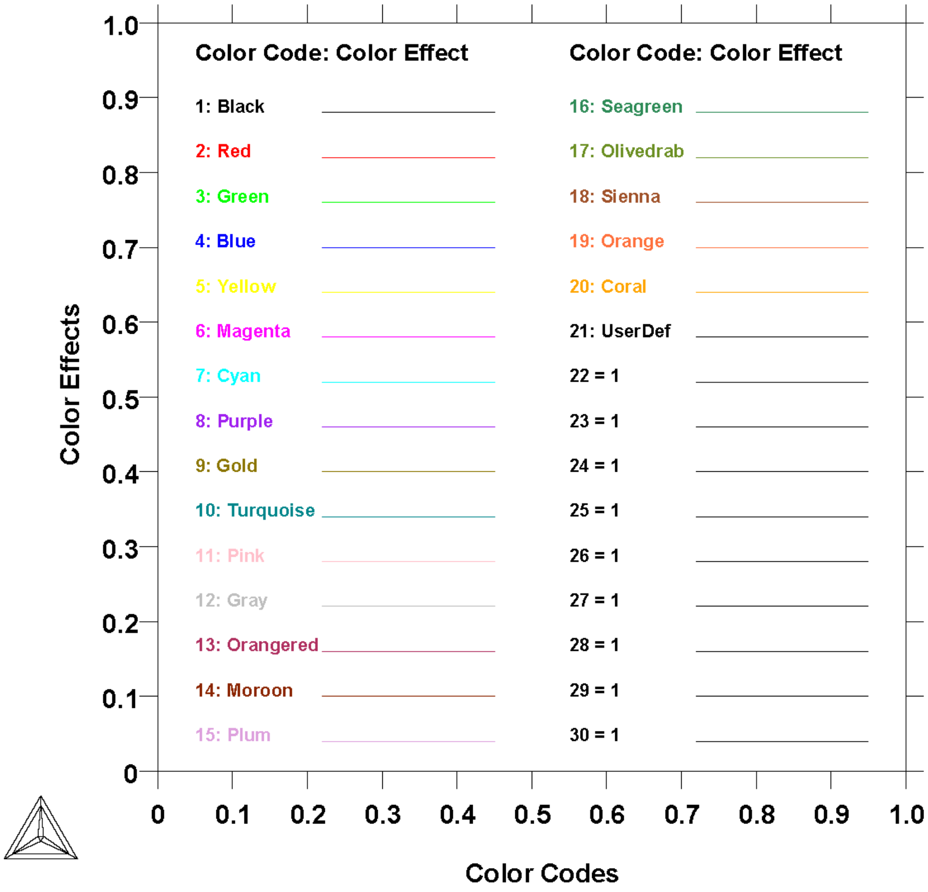
Syntax	`COLOR code`
	`code` is an unsigned integer number (from 0 to 21) identifying the color, or a character string specifying the color.

DIGLIB Color Codes

Code	Color	Equivalent Character
0	Background	Invisible
1	Black	Normal
2	Red	Very_Thick
3	Green	Thin
4	Blue	Thick

Code	Color	Equivalent Character
5	Yellow	Very_Thin
6	Magenta	Dashed
7	Cyan	Dotted
8	Purple	
9	Gold	
10	Turquoise	
11	Pink	
12	Gray	
13	Orangered	
14	Maroon	
15	Plum	
16	Seagreen	
17	Olivedrab	
18	Sienna	
19	Orange	
20	Coral	
21	UserDef	
22 and higher	Any digit larger than 21 has the color effect as 1 (black).	

DIGLIB Color Effects



FONT

FONT redefines the default font setting in the POST-processor.

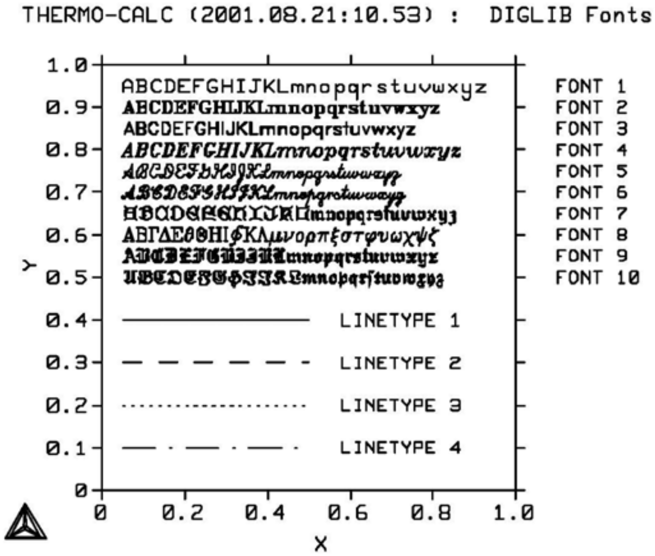
Syntax	`FONT #`
	# is an unsigned integer.

Font Numbers

Number	Font Name
1	Cartographic Roman (the default)
2	Bold Roman script
3	Bold Roman
4	Bold italic
5	Script

Number	Font Name
6	Bold script
7	UNCIAL
8	Bold Greek
9	Gothic English
10	Gothic Greek

Examples of all the DIGLIB fonts and line types



STRING

STRING defines a string containing a text and operation codes (e.g., to change the default font settings).

Syntax	`STRING name text_with_each_character_in_ ^S#^G^F#^U#^D#^R#^L#^N`
	`name` is a valid alphanumeric name (variable) to represent the text including all text formatting codes. It is highly recommended that all the characters in the name are in CAPITAL CASE (e.g. ACA2SO4); otherwise, the defined STRING can be incorrectly plotted. `text_with_each_character_in_^S#^G^F#^U#^D#^R#^L#^N` means the text is coded with each of its characters (and/or numeric numbers) that are formatted with various operators (`^S#`, `^G`, `^F#`, `^U#`, `^D#`, `^R#`, `^L#` and/or `^N`). `#'` are unsigned integers. `^` is the caret character and does not mean a control character. Between an `#` (in an operator) and a numeric number (as a part of the text), there must always be a comma sign (`,`) or the number is not plotted in the text, because the `#` with the number is interpreted as another incorrect #. In some of the commands, `#=0` resets the option to previous (or default) value.

String operation codes in the DIGLIB software

For the PostScript hardcopy fonts, these operation codes are not valid; see *LaTeX Formatting Codes* on page 12:

Operator	Operation
`^S#`	Set character size to size #
`^G`	Set font to Greek
`^F#`	Set font to font number #
`^U#`	Move up # units
`^D#`	Move down # units
`^R#`	Move right # units
`^L#`	Move left # units
`^N`	Do not move, remain at current

Examples

```
STRING Alpha1 ^Ga^F0^D0^S8,1^S0^U0
```

is set to α_1

```
STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0
```

is set to $M_{23}C_6$

```
STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0
```

is set to Ca_2CO_3

TEXT

TEXT outputs, at the current position, the text following the keyword TEXT or the text in the string `string_name` that is defined with *STRING* on page 25.

Syntax	`TEXT text` or `~string_name`
	It is possible to mix ^ operators and previously defined string names using the ~ operator.

FUNCTION

FUNCTION defines and plots a user-defined function.

Syntax	`FUNCTION Y=f(X); start end number_of_XY_pairs; GOC;` `FUNCTION X=f(Y); start end number_of_XY_pairs; GOC;`
	`f(X)` or `f(Y)` are legal mathematical functions of X or Y, understandable by a FORTRAN program. `start` and `end` are unsigned real numbers, and `number_of_XY_pairs` an unsigned integer. `GOC` is a legal graphical operation code as defined with *BLOCK* on page 19.

PCFUNCTION

PCFUNCTION appends a user-defined function to the current path. It is used with *PAINT* below.

Syntax	`PCFUNCTION Y=f(X); start end number_of_XY_pairs; GOC;` `PCFUNCTION X=f(Y); start end number_of_XY_pairs; GOC;`
	`f(X)` or `f(Y)` are legal mathematical functions of X or Y, understandable by a FORTRAN program. `start` and `end` are unsigned real numbers, and `number_of_XY_pairs` an unsigned integer. `GOC` is a legal graphical operation code as defined with *BLOCK* on page 19.

PAINT

PAINT paints the area enclosed by the current path in the current pattern. The current path starts at the last MOVETO given and includes all subsequent DRAWs. This command only works for the PostScript format (as graphical files or on printed hardcopy).

Also see *PCFUNCTION* above.

Syntax	`PAINT <code> <video> <mode>`
	<> denotes optional parameters. To set a new current pattern, supply any or all of the optional parameters. • `<code>` is a single letter 0-9, A-Z or a-t (if `<code>=t`, also supply a space and a number in the range 0.00-1.00). The default is `0`. • `<video>` is a string reading NORMAL (the default) or INVERSE. • `<mode>` is a string reading TRANSPARENT (the default) or OPAQUE.

INCLUDE

INCLUDE adds a file into the current input stream See *Example 5 – Use Included Files for Predefined Symbols* on page 34.

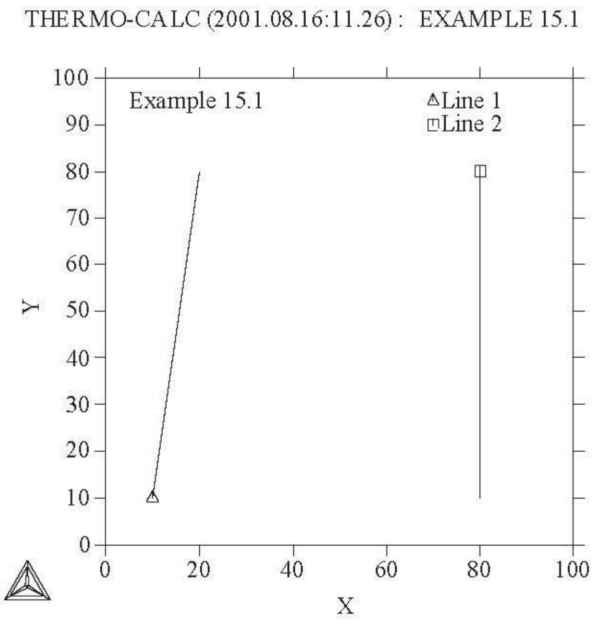
Syntax	`INCLUDE filename`
	`filename` is a legal filename (with its correct path) for the operation system.

Examples of DATAPLOT Files and Outputs

In this section:

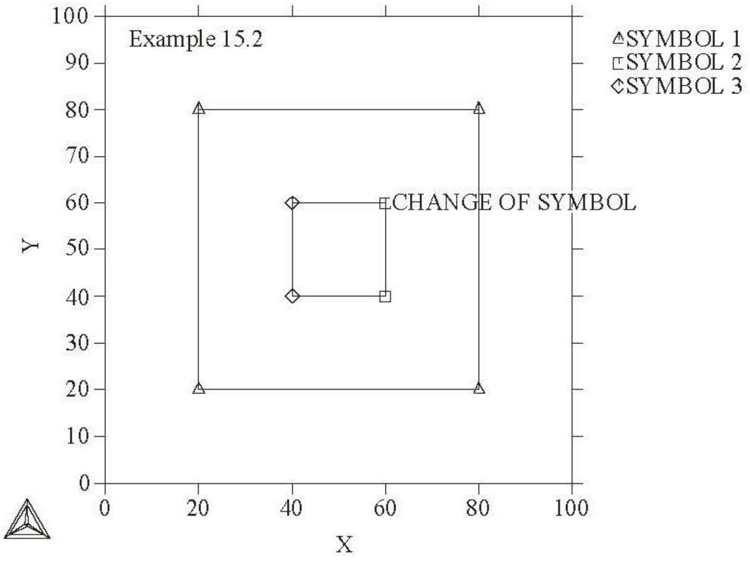
Example 1 – Draw Lines and Symbols

```
$DATAPLOT Example 1
PROLOG 1 EXAMPLE 10<X<100, 0<Y<100
XSCALE0.00000100
YSCALE0.00000100
XTYPE LINEAR YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000
TITLEEXAMPLE 1 XTEXT X
YTEXTY

DATASET 1 Two lines started with two symbols
ATTRIBUTE CENTER
0.050.95 N'Example 1
0.70.95 NS'Line 1
0.70.90 NS2'Line 2 1010S1
2080D
8080S2
8010D
5060
```



Example 2 – Draw Polygons and Symbols

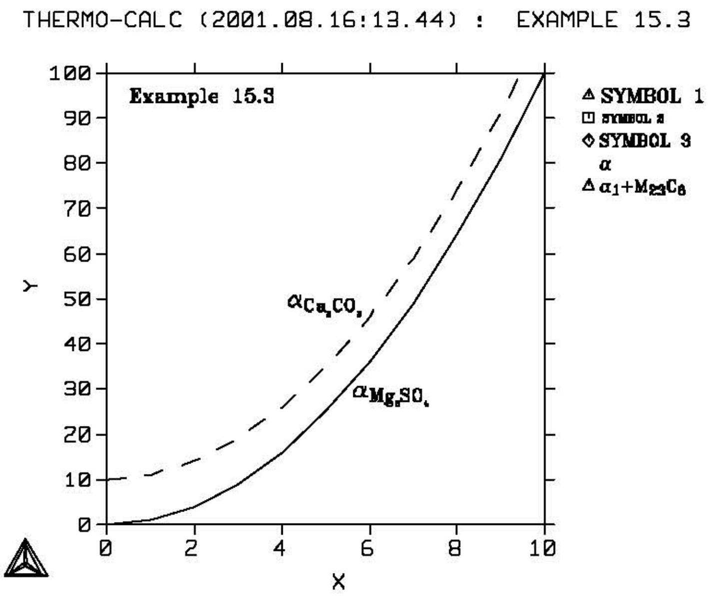
```
$DATAPLOT Example 2
PROLOG 2 EXAMPLE 20<X<100, 0<Y<100
XSCALE0.00000100
YSCALE0.00000100
XTYPE LINEAR YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000
TITLEEXAMPLE 2 XTEXT X
YTEXTY

DATASET 2 Two ploygons with three types of symbols ATTRIBUTE CENTER
CLIP OFF
0.050.95 N'Example 2
1.10.95 NS1'SYMBOL 1
1.10.90 NS2'SYMBOL 2
1.10.85 NS3'SYMBOL 3
BLOCK X=C1; Y=C2; GOC=C3,DSWA
4040M
4060
6060S2'CHANGE OF SYMBOL
6040
4040S0
BLOCKEND
BLOCK X=C1*100; Y=C2*100; GOC=C3,DSWA 0.20.2 MS1
0.20.8
0.80.8
0.80.2
0.20.2
BLOCKEND
```



Example 3 – Using Strings and Various Line Types

```
$DATAPLOT Example 3
PROLOG 3 EXAMPLE 3  0<X<10, 0<Y<100
XSCALE0.0000010
YSCALE0.00000100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000
TITLE EXAMPLE 3 XTEXT X
YTEXT Y
DATASET 3 Draw curves; plot formatted texts and symbols
$Define some strings: STRING BCC ^Ga^F0
STRING BCC1 ^Ga^F0^D0^S8,1^S0^U0
STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0
STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0 STRING AMG2SO4
^Ga^F0^D0^S8Mg^D0^S4,2^S0^U0^S8SO^D0^S4,4^S0^U0
$ Note: if as PostScript output:
$STRING BCC !a
$STRING BCC1 !a^do1$
$STRING M23C6 M^do23$C^do6$
$STRING ACA2CO3 !a^doCa^do2$^doCO^do3$
$STRING AMG2SO4 !a^doMg^do2$^doSO^do4$ ATTRIBUTE CENTER
```

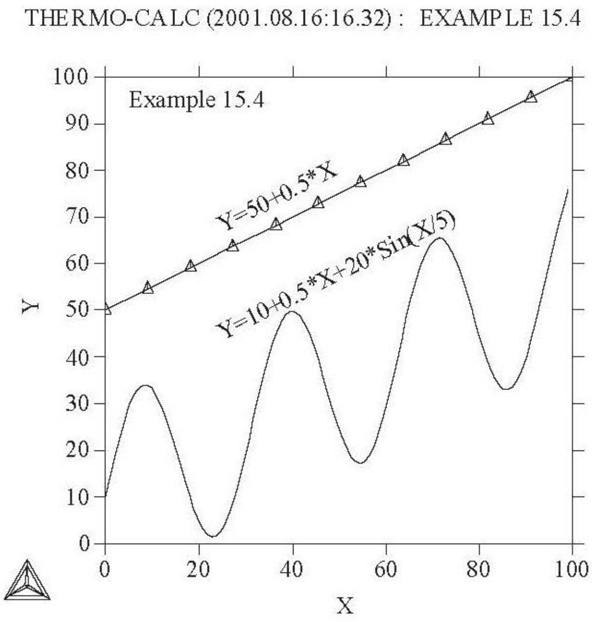
```
CLIP OFF FONT 2
0.05  0.95 N'Example 3
1.10.95 NS1'SYMBOL 1 CHARSIZE 0.2
1.10.90 NS2' SYMBOL 2 CHARSIZE 0.3
1.10.85 NS3'SYMBOL 3 1.10.80 N' ~BCC
1.10.75 NS1'~BCC1+~M23C6
SYMBOLSIZE 0.4
CHARSIZE 0.4
0.41  0.50 N'~ACA2CO3
0.56 0.30 N'~AMG2SO4 CLIP ON
LINETYPE 1
BLOCK X=C1; Y=C1*C1; GOC=C2, DWA
1 2 3  4  5  6  7  8  9           10
BLOCKEND LINETYPE 2
BLOCK X=C1; Y=C1*C1+10; GOC=C2, DWA
0 M 1 2 3  4  5  6  7  8  9           10
BLOCKEND
0 M
```



Example 4 – Draw Curves Defined by Functions

```
$DATAPLOT Example 4
PROLOG 4 EXAMPLE 40<X<100, 0<Y<100
```

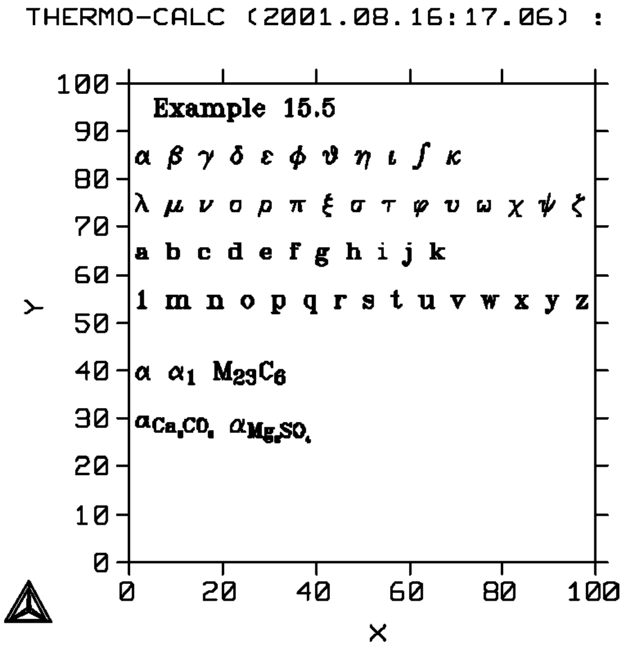
```
XSCALE0.00000100
YSCALE0.00000100
XTYPE LINEAR YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000
TITLEEXAMPLE 4 XTEXT X
YTEXTY
DATASET 4 Plot two functions as lines: ATTRIBUTE CENTER
0.050.95 N'Example 4
$ Draw two lines defined by FUNCTIONS:
FUNCTION Y=10+0.5*X+20*Sin(X/5); 0 100 100; DWA;
FUNCTION Y=50+0.5*X; 0 100 10; DS1WA;
$ Write funtions beside the lines:
$Note the real rotation angle (27 degree) can be seen
$only on the PostScript hardcopy! 0.250.68 N'^RO27Y=50+0.5*X
0.250.45 N'^RO27Y=10+0.5*X+20*Sin(X/5)
```



Example 5 – Use Included Files for Predefined Symbols

```
$DATAPLOT Example 5
PROLOG 5 EXAMPLE 50<X<100, 0<Y<100
XSCALE0.00000100
YSCALE0.00000100
```

```
XTYPE LINEAR YTYPE LINEAR

XLENGTH11.5000

YLENGTH11.5000

TITLEEXAMPLE 5 XTEXT X

YTEXTY

DATASET 5 Write characters in various fonts, and defined symbols FONT 2

INCLUDE <DATAPLOT-EXAMPLE-PATH>INCLUDE.EXP ATTRIBUTE CENTER

0.050.95 N'Example 5 CLIP OFF

0.010.85 N'~TEST1A

0.010.75 N'~TEST1B

0.010.65 N'~TEST2A

0.010.55 N'~TEST2B

0.010.40 N'~BCC ~BCC1 ~M23C6

0.010.30 N'~ACA2CO3 ~AMG2SO4
```



The INCLUDE.EXP file has the following content:

```
STRING TEST1A ^Ga b c d e f g h i j k^F0

STRING TEST1B ^Gl m n o p q r s t u v w x y z^F0 STRING TEST2Aa b c d e f g h i j k

STRING TEST2B1 m n o p q r s t u v w x y z STRING BCC ^Ga^F0

STRING BCC1 ^Ga^F0^D0^S8,1^S0^U0

STRING BCC2 ^Ga^F0^D0^S8,2^S0^U0 STRING FCC ^Gc^F0
```

```
STRING FCC1 ^Gc^F0^D0^S8,1^S0^U0 STRING FCC2 ^Gc^F0^D0^S8,2^S0^U0

STRING L Liquid STRING SIGMA ^Gs^F0 STRING MU ^Gm^F0 STRING LAVES ^Gl^F0 STRING CHI
^Gx^F0 STRING KSI ^Gr^F0

STRING MCETA ^S12^Gh^F0^S0 STRING M2CM^D0^S8,2^S0^U0C STRING M2CT M^D0^S10,2^S0^U0C
STRING M6CM^D0^S8,6^S0^U0C

STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0 STRING M7C3
M^D0^S8,7^S0^U0C^D0^S8,3^S0^U0 STRING M3C2 M^D0^S8,3^S0^U0C^D0^S8,2^S0^U0 STRING MC1-X
MC^D0^S8,1-x^S0^U0

STRING XC x^D0^S7,C^S0^U0 STRING XFE x^D0^S7,Fe^S0^U0 STRING XMO x^D0^S7,Mn^S0^U0
STRING XW x^D0^S7,W^S0^U0 STRING UW ~XW/(~XMO+~XW)

STRING ac a^D0^S7,C^S0^U0 STRING ACC a^D0^S7,C^S0^U0

STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0 STRING AMG2SO4
^Ga^F0^D0^S8Mg^D0^S4,2^S0^U0^S8SO^D0^S4,4^S0^U0

$ Note: if as PostScript output:

$STRING TEST1A !a !b !c !d !e !f !g !h !i !j !k^fo27

$STRING TEST1B !l !m !n !o !p !q !r !s !t !u !v !w !x !y !z^fo27

$STRING TEST2Aa b c d e f g h i j k

$STRING TEST2B1 m n o p q r s t u v w x y z

$STRING BCC !a

$STRING BCC1 !a^do1$

$STRING BCC2 !a^do2$

$STRING FCC !c

$STRING FCC1 !c^do1$

$STRING FCC2 !c^do2$

$STRING L Liquid

$STRING SIGMA !s

$STRING MU !m

$STRING LAVES !l

$STRING CHI !x

$STRING KSI !r

$STRING MCETA !h

$STRING M2CM^do2$C

$STRING M2CT M^do2$C

$STRING M6CM^do6$C

$STRING M23C6 M^do23$C^do6$

$STRING M7C3 M^do7$C^do3$

$STRING M3C2 M^do3$C^do2$

$STRING MC1-X MC^do1-x$
```

```
$STRING XC x^doC$
$STRING XFE x^doFe$
$STRING XMO x^doMo$
$STRING XW x^doW$
$STRING UW ~XW/(~XMO+~XW)
$STRING ac a^doC$
$STRING ACC a^doC$
$STRING ACA2CO3 !a^doCa^do2$^doCO^do3$
$STRING AMG2SO4 !a^doMg^do2$^doSO^do4$
```

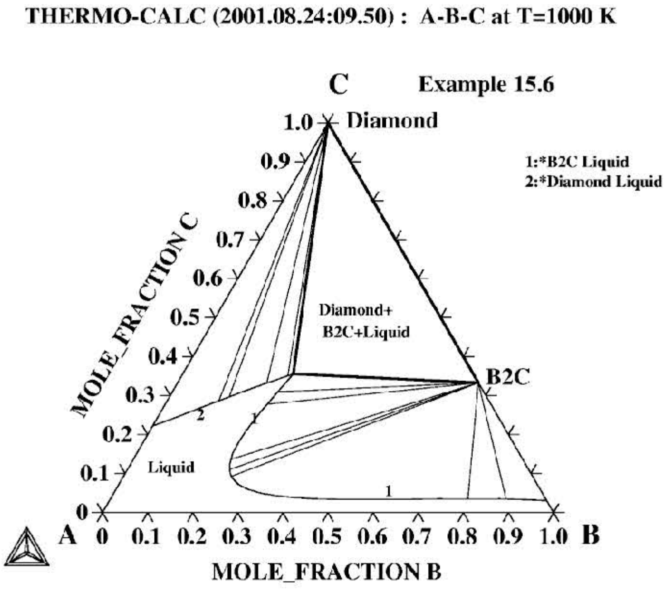
Example 6 – Plot Triangular Diagrams for Ternary Systems

```
$DATAPLOT Example 6
PROLOG 6 EXAMPLE 6  0<X<0.969224, 0<Y<1.00000
XSCALE0.000000.969224
YSCALE0.307492E-011.00000
XTYPE LINEAR YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000 TITLE A-B-C at T=1000 K XTEXT MOLE_FRACTION B YTEXT  MOLE_FRACTION C
DIAGRAM_TYPE TRIANGULAR YES YES
DATASET 6 Plot a ternary phase diagram CLIP OFF
0.70 0.95 N'Example 6 0.85  0.30 N'B2C
0.54 0.87 N'Diamond CHARSIZE 0.25
1.4E+01  1.10E+01 MVA'1:*B2C Liquid
1.4E+01  1.05E+01 MVA'2:*Diamond Liquid
0.10  0.10 N'Liquid
0.48  0.45 N'Diamond+
0.48 0.40 N' B2C+Liquid 5.80E-01  5.40E-02 MWA' 1
1.90E-01  2.40E-01 MWA' 1
0.65E-01  2.50E-01 MWA' 2
CHARSIZE 0.45
-0.10  -0.05 N'A
1.06  -0.05 N'B
0.500.95 N'C
CHARSIZE 0.35
$$ Calculated A-B-C Phase Equilibrium Data:
$ PHASE REGION FOR:
$F0 LIQUID
```

```
$E DIAMOND_A4
$F0 B2C
$ INVARIANT EQUILIBRIUM COLOR2
BLOCK X=C1; Y=C2;GOC=C3,WAD; 2.4555855989E-013.5568857193E-01M
0.0000000000E+009.9999523163E-01
2.4555855989E-013.5568857193E-01M
6.6666668653E-013.3333334327E-01
0.0000000000E+009.9999523163E-01M
6.6666668653E-013.3333334327E-01 COLOR1
BLOCKEND
$ PHASE REGION FOR:
$E LIQUID
$F0 B2C
BLOCK X=C1; Y=C2;GOC=C3,WAD;
$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)
2.2030337155E-011.2340000272E-01M
2.2632879019E-011.1058768630E-01
2.3371633887E-019.9345825613E-02
2.4253317714E-018.9345827699E-02
2.6429468393E-017.2744041681E-02
2.8429466486E-016.2814079225E-02
2.9617273808E-015.8319382370E-02
3.2811737061E-014.9470417202E-02
3.6353862286E-014.3130427599E-02
3.9895987511E-013.8979098201E-02
4.5209178329E-013.5266116261E-02
5.2293431759E-013.3152002841E-02
6.1148744822E-013.3077053726E-02
6.4690870047E-013.3490389585E-02
6.8232995272E-013.4017231315E-02
7.3546189070E-013.4814555198E-02
7.5317251682E-013.5033416003E-02
8.0630439520E-013.5373892635E-02
8.5943627357E-013.4983776510E-02
9.1256815195E-013.3575300127E-02
9.6747112274E-013.0857827514E-02
```

```
9.6922445297E-013.0749246478E-02

2.2030337155E-011.2340000272E-01M

2.1294665337E-011.5308913589E-01

2.1171525121E-011.8851040304E-01

2.1532440186E-012.2393165529E-01

2.2180187702E-012.5935292244E-01

2.2992117703E-012.9477417469E-01

2.3888295889E-013.3019542694E-01

2.4555855989E-013.5568857193E-01

$ PLOTTED COLUMNS ARE : X(B2C,B) and X(B2C,C) 6.6666668653E-013.3333334327E-01M

6.6666668653E-013.3333334327E-01

$ TIELINES COLOR3

6.6666668653E-013.3333334327E-01M

8.7775242329E-013.4625384957E-02

6.6666668653E-013.3333334327E-01M

7.9250496626E-013.5342670977E-02

6.6666668653E-013.3333334327E-01M

2.4555824697E-013.5568737984E-01

6.6666668653E-013.3333334327E-01M

2.3944084346E-019.2542596161E-02

6.6666668653E-013.3333334327E-01M

2.3359020054E-013.0954307318E-01

6.6666668653E-013.3333334327E-01M

2.2585247457E-012.7766343951E-01

6.6666668653E-013.3333334327E-01M

2.1618695557E-011.3621240854E-01

2.2632879019E-011.1058768630E-01M

6.6666668653E-013.3333334327E-01 COLOR1

BLOCKEND

$ PHASE REGION FOR:

$F0 DIAMOND_A4

$E B2C

BLOCK X=C1; Y=C2;GOC=C3,WAD;

$ PLOTTED COLUMNS ARE : X(DIAMOND_A4,B) and X(DIAMOND_A4,C)
0.0000000000E+009.9999523163E-01M

0.0000000000E+009.9999976158E-01 BLOCKEND
```

```
$ PHASE REGION FOR:
$E LIQUID
$F0 DIAMOND_A4
BLOCK X=C1; Y=C2;GOC=C3,WAD;
$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)
2.45558E-01  3.55688E-01 M
2.02635E-01 3.34830E-01
1.62439E-01 3.13753E-01
1.22439E-01 2.91531E-01
8.24390E-02 2.68542E-01
4.24390E-02 2.45480E-01
2.43905E-03 2.23138E-01
2.49999E-07 2.21816E-01
$ TIELINES COLOR3
0.00000E+00  9.99995E-01 M
2.35291E-01 3.50859E-01
0.00000E+00  9.99994E-01 M
1.98265E-01 3.32609E-01
0.00000E+00  9.99994E-01 M
1.32400E-01 2.97160E-01
0.00000E+00  9.99993E-01 M
1.14399E-01 2.86953E-01 BLOCKEND
```



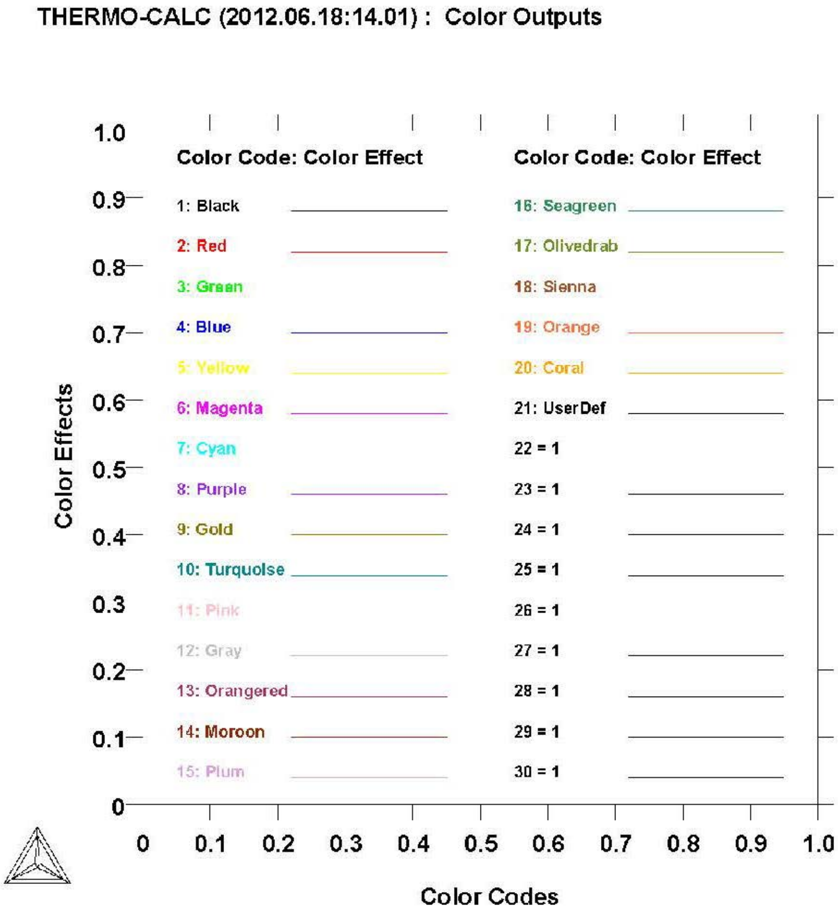
Example 7 – Color Codes and Effects

```
$DATAPLOT Color Codes & Color Effects

PROLOG 10 Color Codes  0<X<1.0, 0<Y<1.0

XSCALE0.01.0

YSCALE0.01.0

XTYPE LINEAR

YTYPE LINEAR

XLENGTH11.5000

YLENGTH11.5000

TITLE Color Outputs XTEXT Color Codes YTEXT  Color Effects

DATASET 10 Various Color Codes for Color Outputs: CHARSIZE 0.3

LINETYPE 1

BLOCK X=C1; Y=C2;GOC=C3,WAD;

0.05  0.95 MNA'Color Code: Color Effect

0.55 0.95 MNA'Color Code: Color Effect CHARSIZE 0.25

COLOR 1

0.05 0.88 MNA'1: Black CLIP ON

0.22  0.88 M

0.45 0.88

CLIP OFF COLOR 2

0.05 0.82 MNA'2: Red CLIP ON

0.22  0.82 M

0.45 0.82

CLIP OFF COLOR 3

0.05 0.76 MNA'3: Green CLIP ON

0.22  0.76 M

0.45 0.76

CLIP OFF COLOR 4

0.05 0.70 MNA'4: Blue CLIP ON

0.22  0.70 M

0.45 0.70

CLIP OFF COLOR 5

0.05 0.64 MNA'5: Yellow CLIP ON

0.22  0.64 M

0.45 0.64

CLIP OFF COLOR 6
```

```
0.05 0.58 MNA'6: Magenta CLIP ON

0.22  0.58 M

0.45 0.58

CLIP OFF COLOR 7

0.05 0.52 MNA'7: Cyan CLIP ON

0.22  0.52 M

0.45 0.52

CLIP OFF COLOR 8

0.05 0.46 MNA'8: Purple CLIP ON

0.22  0.46 M

0.45 0.46

CLIP OFF COLOR 9

0.05 0.40 MNA'9: Gold CLIP ON

0.22  0.40 M

0.45 0.40

CLIP OFF COLOR 10

0.05 0.34 MNA'10: Turquoise CLIP ON

0.22  0.34 M

0.45 0.34

CLIP OFF COLOR 11

0.05 0.28 MNA'11: Pink CLIP ON

0.22  0.28 M

0.45 0.28

CLIP OFF COLOR 12

0.05 0.22 MNA'12: Gray CLIP ON

0.22  0.22 M

0.45 0.22

CLIP OFF COLOR 13

0.05 0.16 MNA'13: Orangered CLIP ON

0.22  0.16 M

0.45 0.16

CLIP OFF COLOR 14

0.05 0.10 MNA'14: Moroon CLIP ON

0.22  0.10 M

0.45 0.10

CLIP OFF COLOR 15
```

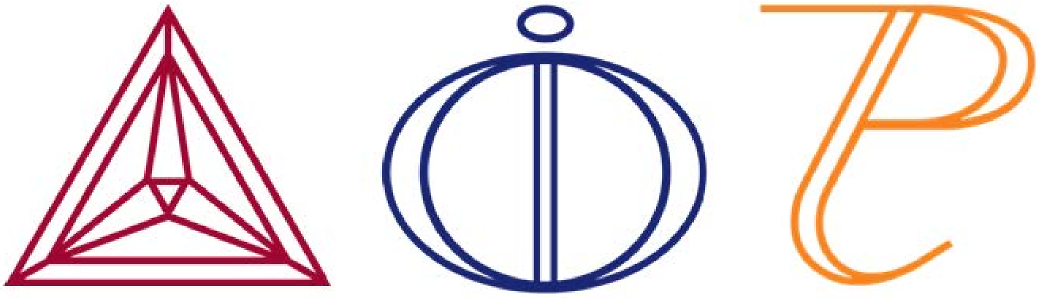
```
0.05 0.04 MNA'15: Plum CLIP ON
0.22  0.04 M
0.45 0.04
CLIP OFF COLOR 16
0.55 0.88 MNA'16: Seagreen CLIP ON
0.72  0.88 M
0.95 0.88
CLIP OFF COLOR 17
0.55 0.82 MNA'17: Olivedrab CLIP ON
0.72  0.82 M
0.95 0.82
CLIP OFF COLOR 18
0.55 0.76 MNA'18: Sienna CLIP ON
0.72  0.76 M
0.95 0.76
CLIP OFF COLOR 19
0.55 0.70 MNA'19: Orange CLIP ON
0.72  0.70 M
0.95 0.70
CLIP OFF COLOR 20
0.55 0.64 MNA'20: Coral CLIP ON
0.72  0.64 M
0.95 0.64
CLIP OFF COLOR 21
0.55 0.58 MNA'21: UserDef CLIP ON
0.72  0.58 M
0.95 0.58
CLIP OFF COLOR 22
0.55 0.52 MNA'22 = 1 CLIP ON
0.72  0.52 M
0.95 0.52
CLIP OFF COLOR 23
0.55 0.46 MNA'23 = 1 CLIP ON
0.72  0.46 M
0.95 0.46
CLIP OFF
```

```
BLOCKEND
```


THERMO-CALC (2012.06.18:14.01) : Color Outputs
Color Code: Color Effect
1: Black
2: Red
3: Green
4: Blue
5: Yellow
6: Magenta
7: Cyan
8: Purple
9: Gold
10: Turquoise
11: Pink
12: Gray
13: Orangered
14: Moroon
15: Plum
Color Code: Color Effect
16: Seagreen
17: Olivedrab
18: Sienna
19: Orange
20: Coral
21: UserDef
22 = 1
23 = 1
24 = 1
25 = 1
26 = 1
27 = 1
28 = 1
29 = 1
30 = 1
Color Effects
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Color Codes
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Database Manager User Guide

Version 2016b



Thermo-Calc Software

Introduction to the Database Manager Guide

In this section:

Thermodynamic and Kinetic/Mobility Databases

This guide describes how to define and construct a thermodynamic or kinetic database. It includes details about the data structures and formats of the Thermo-Calc databases as well as the Diffusion Module (DICTRA) database-extensions.

The Thermo-Calc databases are created and maintained in the Thermo-Calc Database Format (TDB) which is an international standard for the CALPHAD-type thermodynamic calculations and kinetic simulations. This document gives a full description of the TDB format (with the Diffusion Module (DICTRA) database extension) and is a comprehensive guide about how to create and manage a Thermo-Calc (and Diffusion Module (DICTRA)) database.

Usually, a Thermo-Calc or Diffusion Module (DICTRA) database is constructed as a single text file with an extension of TDB, for example, `PAQS2setup.TDB`. For some databases (especially large databases used with older versions of Thermo-Calc or Diffusion Module (DICTRA)) a database may consist of one primary-definition file (`***setup.TDB`) and several additional-definition TDB files (such as `***param.TDB`, `***funct.TDB`, `***refer.TDB`, etc. These are built for a variety of defined parameters, functions, references and so forth, and are linked to the `***setup.TDB` file through the correct use of the *TYPE_DEFINITION* on page 18 and/or *FTP_FILE* on page 21 commands inside the `***setup.TDB` file.

With Thermo-Calc, Precipitation Module (TC-PRISMA) and Thermo-Calc Software Development Kits (SDKs), you can code everything into a single *****setup.TDB** file for a database at any scale.

Initialization of the DATA Module

The following explains how a database initiation file (or a database directory file) is constructed to work with the DATA module. When you start, DATA looks for this file that has information about the available predefined databases.

The *database initiation file* is called:

- Windows: `TC_INITD.TDB` (or `TC_INITD`)
- Linux/UNIX: `initd.tdb`

You can have your own file, but it is more efficient to define an environment variable with the default name as above, and then during installation, translate it to a common initiation file name. The common file is automatically copied by the Thermo-Calc installation script to the following directories:

- Windows: `\DATA\` under the directory defined by the `TCPATH` parameter
- Linux/UNIX:`/data/` under the directory defined by the `TC_DATA` parameter.

The database manager can find the file on a local computer (independent installations) or a connected server (server installations).

When editing or modifying the definitions of initiation parameters (including short-names, paths and subdirectories, database definition file names, and instructive database descriptions) for the available databases in the database initiation file a specific format is used with the fields:

- The first field gives the abbreviated name for the database (to a maximum of five characters)
- The second field specifies a path and filename (maximum 78 characters) containing the database path definition and the actual database definition (*setup*) file name, where the extension is either `TDB` (which stands for original textual TDB file) or `TDC` (which is encrypted from the original TDB file). There are differences between platforms with respect to entering parameters as listed in the table.
- The third field (maximum 60 characters) details an optional full name (and version/subversion numbers) for the brief database description.

Initiation Parameter Examples

Parameter	**Windows**	**Linux/Unix**
The `setup` file name must consist of a main part and an extension of a maximum of three characters:	For example, `SSOL5SETUP.TDB`	For example, `ssol5setup.tdb`
Database path definition	Use a back-slash `\`	Use a forward-slash `/`
All databases should be normally located in subdirectories that are under the directory defined by the:	`TCPATH` parameter or under its subdirectory `\DATA\`	`TC_DATA` parameter or under its subdirectory `/data/`

Each entry record (i.e. for a single database) must finish with an exclamation mark !. There should be no spaces or commas within the first and second fields since these characters are taken as field separators, while spaces or commas can be used in the third field.

You can write each database entry on one or two lines (up to the!), it is recommended that the third field is added as follows:

- Windows: on the same line as the first and second fields.
- Linux/UNIX: on the following line.

The following are examples of an initiation file defining two databases named SSOL6 and TCFE8.

Windows

```
SSOL6 TCPATH\DATA\SSOL6\SSOL6SETUP.TDC  SGTE Solutions Database
version 6.0 !

TCFE8 TCPATH\DATA\TCFE8\TCFE8SETUP.TDC  TCS Steels/Fe-Alloys Database
version 8.0 !
```

Linux/UNIX

```
ssol5 TC_DATA/data/ssol5/ssol5setup.tdc

     SGTE Solutions Database version 5.1  !

Tcfe8 TC_DATA/data/tcfe8/tcfe8setup.tdc

     TCS Steels/Fe-Alloys Database version 8.0 !
```

The Database Definition File and Keywords

In this section:

Database Definition File Syntax

The database definition (*.TDB) file (normally named `***setup.TDB`) consists of a set of keyword codes each followed by one or several parameters (arguments).

- A complete keyword entry must end with an exclamation mark (!).
- A single keyword entry can be up to 2000 characters long. However, the maximum length of a line in an *.TDB file is 78 characters--it may be necessary to continue the keyword parameter (arguments) on several lines. The ! must be at the end of the last line.
- It is recommended to always have at least one empty space at the beginning of each continuation line for the keyword parameters (arguments); otherwise, the DATA module can misunderstand the parameters (or arguments), or issue an error message.
- The keyword and its various parameters (arguments) are separated by a space or a comma.
- A dollar sign ($) in the first position of the line indicates that the line is a comment line, which is ignored by the DATA module.

When the database is selected the DATA module only reads the database definition file (***setup.TDB) once, from beginning to end. The DATA module checks continuously when reading the definition file. This implies that (nearly) everything must be declared or defined before it is used in any other way.

For example, if the GRAPHITE phase is to be included in the database definition, the element C (carbon) and the phase GRAPHITE must be defined before declaring that carbon dissolves in graphite. This definition order is necessary to build the internal data structure acceptable by the DATA module (during its consistency checking).

This topic gives a description of the available keywords and the appropriate arguments. A basic knowledge of the Gibbs Energy System (GIBBS) module is assumed.

This syntax is used:

```
KEYWORD [arg.1]*# [arg.2]*## {optional arg.3}!
```

The keywords are written in full length but can be abbreviated as long as the abbreviation is unique. A keyword may have syntax consisting of several arguments and optional arguments. The number, # or ##, in the notation, [...]*# or [...]*##, indicates an argument with a maximum length of # ASCII characters.

Arguments within square brackets `[...]` must always be given, but are optional when enclosed in curly brackets `{...}`.

ELEMENT

```
ELEMENT [element name]*2 [ref. state]*24 [mass] [H298] [S298] !
```

The *element name* (maximum two characters) is the one found in the periodic chart but there are no naming restrictions. However, the GIBBS module only recognizes UPPER-case element names (if the `Upper Case Mode` is selected by the GIBBS command *REINITIATE* on page 83), which means that lower-case (if defined in a database) is automatically converted to UPPER-case by the DATA/GIBBS module.

The elements are automatically entered as species using the same names of the elements. If, for example, the species corresponding to FE needs to be named FE1, you can define the species as FE1, which results in an element named FE and a species named FE1. Vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase), need to be entered as special elements for correct handling by the DATA module.

The *reference (ref.) state* (maximum 24 characters) is the stable phase (at 298.15 K and 1 bar) that should contain this element and be used as the reference state for all element thermodynamic data. The *mass*, given in gram per mole, is used in various calculation programs and should always be given the correct value. *H298* and *S298* denote the enthalpy and entropy difference between 0 and 298.15 K for the element in SI units. If these are unknown, the values can be set to zero. All this information (reference state, H298 and S298) define the SER (Stable Element Reference state).

Examples

```
ELEMENT /- ELECTRON_GAS       0.0   0.0   0.0 !

ELEMENT VA VACUUM             0.0   0.0   0.0 !

ELEMENT ZE UNIT_CHARGE        0.0000000001  0.0   0.0 !

ELEMENT AL FCC_A1             26.98154 4577.296 28.3215 !

ELEMENT C  GRAPHITE           12.011  1054.0    5.74 !

ELEMENT FE BCC_A2             55.847  4489     27.28 !

ELEMENT O  1/2_MOLE_O2(G)     15.9994 4341    102.5158 !

ELEMENT TI HCP_A3             47.88   4810     30.648 !

ELEMENT ZR HCP_A3             91.224  5566.27  39.181 !

ELEMENT ZY DUMMY               1         1         1 !
```

SPECIES

```
SPECIES [species name]*24 [stoichiometric formula] !
```

This keyword defines species in the data structure. Every *species name* (maximum 24 characters) must be unique. The species are built from the predefined set of elements in the stoichiometric formula. If an undefined element is referenced, DATA displays an error message and the data structure is probably damaged.

The species names do not have to be the same as the stoichiometry formula, although in general this is recommended. The elements are automatically entered as species using the same names of the elements.

You can define a species name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case species names.

When naming the species in a database, use special characters (such as +, -, _, / and .) in species names. Avoid using other special characters (such as `(` and `)`).

The *stoichiometric formula* is written with a simplified chemical notation, in which the chemical elements should always be given in UPPER-case and in any preferred order, and the stoichiometric coefficients are written in either real numerical factors or integer digits.

It is important that the numerical factor of `1` is not left out. Subgroups are not allowed in a stoichiometry formula; however, while specifying the stoichiometry formula for a specific species in a database, you can specify it in a way that some elements (always together with the corresponding partial stoichiometric coefficients) are repeated (as in the examples below).

Examples

```
SPECIES AL2O3      AL2O3 !
SPECIES Silica     SI1O2 !
SPECIES NaSb_6OH   NA1SB1O6H6 !
SPECIES FE+2        FE/+2 !
SPECIES SB-3        SB/-3 !
SPECIES AlCl2/3            AL.33333CL.666667 !
SPECIES AL1CL1H2O2         AL1CL1H2O2 !
SPECIES AlCl3_3H2O         AL1CL3H6O3 !
SPECIES AlO2H2Cl.H6O3      AL1O2H2CL1H6O3 !
SPECIES AlCl2-OH.3H2O      AL1CL2O1H1H6O3 !
SPECIES AlCl2OH.3Water     AL1O1H1CL2H6O3 !
```

PHASE

```
PHASE [phase name]*24 [data-type code]*8 [numb. subl.] [sites in
subl. 1] [sites in subl. 2] etc... {auxiliary text string} !
```

This keyword defines a phase and its properties (except for what species are allowed to enter it and for its parameters).

The *phase name* (maximum 24 characters) must be unique; otherwise the DATA module sees it as an attempt to redefine a previously defined phase. This causes DATA to display an error message and ignore the rest of the line. A phase name can be suffixed by an underscore (_and letters to identify the physical state(s) or structure type(s) of the phase.

Examples of Recommended Suffixes

Suffix	Definition
`ABC_S`	The `ABC` phase in solid state.
`ABC_S2`	The `ABC` phase in solid state 2.
`ABC_S3`	The `ABC` phase in solid state 3.
`ABC_LT`	The `ABC` phase in solid state at low temperatures.
`ABC_HT`	The `ABC` phase in solid state at high temperatures.
`ABC_L`	The `ABC` phase in liquid state.
`ABC_LIQ`	The `ABC` phase in liquid state.
`FCC_A1`	The `FCC` phase in disordered structure type A1.
`FCC_L12`	The `FCC` phase in ordered structure type L12.

The *phase name* can also be attached with a colon sign (`:`) and a letter for a legal GIBBS phase-type code (e.g. `IONIC_LIQ:Y` and `GAS:G`).

GIBBS Phase-type Codes

Code	Definition
`G`	Bit set for a gaseous mixture phase.
`A`	Bit set for an aqueous solution phase.
`Y`	Bit set for an ionic liquid solution phase (specially treated by the Ionic Two-Sublattice Liquid Model).
`L`	Bit set for a liquid solution phase (but not A (aqueous) or Y (ionic liquid)).
`I`	Bit set for a phase with charged species (but not G (gaseous), A (aqueous) or Y (ionic liquid)).
`F`	Bit set for an ordered FCC or HCP solution phase using the *Four Substitutional-Sublattice Ordering Model* (additionally, such a phase can also have interstitial sublattices).
`B`	Bit set for an ordered BCC solution phase using the *Four Substitutional-Sublattice Ordering Model* (additionally, such a phase can also have interstitial sublattices).

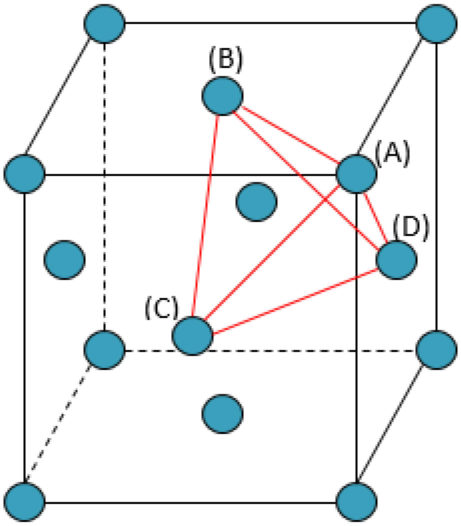
Other invalid characters (e.g. `M` or `P`) are eventually treated, together with the colon (:) as a part of a phase name.

A `G` phase (gaseous mixture) or an `A` phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and an `L` phase (ordinary liquid solution) is normally (but not always) modelled as a substitutional phase without sublattice, too.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours, as shown.

FCC Unit Cell Example

An FCC unit cell with the lattice positions indicated that correspond to the G (FCC,A:B:C:D) end member. All lattice positions are equivalent for a four substitutional-sublattice ordering model.



A *Normal 4-Sublattice Model* requires that all the `G` parameters for each of the end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option `F` means that the `G` parameters need be given only once. The possible permutations are handled automatically.

Additional Clarification

An `A–B` binary solution phase (with the element A located on one sublattice site and `B` on the other three sublattice sites) treated by the Normal 4-Sublattice Model has to have four `G` parameters for four end-members, i.e.

- G(phase,A:B:B:B)
- G(phase,B:A:B:B)

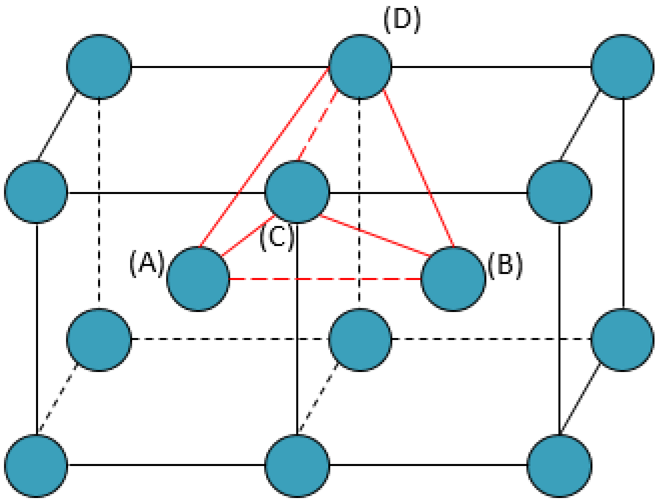
- G(phase,B:B:A:B, and
- G(phase,B:B:B:A)

This is because in the general case these `G` parameters can be different from each other. But for the FCC and HCP orderings, they are identical and thus all `G` parameters of such end-members need to be given only once, and the possible permutations are then automatically handled by the GIBBS module. Also, only one of the identical permutations is listed; in this example, `G(phase,A:B:B:B)` where it is alphabetically the first in the list of permutations. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

For ordered BCC phases, the phase-type option `B` means the same thing but it is more complicated since the 4-substitutional-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours as shown:

BCC Unit Cell Example

Two BCC unit cells with the lattice positions indicated that correspond to the G (BCC,A:B:C:D,0) end member. Lattice positions (A) and (B) are equivalent, as are lattice positions (C) and (B) for a four substitutional-sublattice ordering model.



For an end member described by the parameter `G (phase,A:B:C:D)` A and B are next nearest neighbours, as are C and D. And the nearest neighbours of A (or B) are C and D. Thus, for an `A–B` binary solution phase (with the element A located on two sublattice sites and `B` on two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the `G(phase,A:A:B:B)` term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the `G (phase,A:B:A:B)` term has two nearest neighbour bonds between A and B atoms and three next nearest neighbour bonds.

The first end-member (described by the `G(phase,A:A:B:B)` term) represents B2-ordering and the second (described by the `G(phase,A:B:A:B)` term) stands for B32-ordering. There are two permutations of the `G(phase,A:A:B:B)` term and four permutations of the `G(phase,A:B:A:B)` term, automatically conducted in the *Four Substitutional-Sublattice Ordering Model*. If you enter the unary, binary, ternary and quaternary parameters you are dealing with 1, 6, 21, 55 parameters for BCC:B, 1, 5, 15, 35 parameters for FCC:F and 1, 16, 81, 256 parameters for phases without F/B.

An additional feature with the phase-type options `F` and `B` is that a composition set that represents the solution phase has a suffix (indicating what ordering the phase has) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams).

Such suffix indications can be:

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
`FCC PHASE`	`FCC_A1`	`FCC_L12`
		`FCC_L10`
`BCC PHASE`	`BCC_A2`	`BCC_B2`
		`BCC_B32`
		`BCC_D03`
		`BCC_L21`
`HCP PHASE`	`HCP_A3`	`HCP_D019`
		`HCP_B19`

If you want to convert an existing database TDB-file to use the F/B feature, add the phase-type code to the corresponding phase name in the PHASE and CONSTITUENT commands in the TDB-file, then when running the LIST_DATA command in the GES module. The created database file is in this less verbose format.

The *data-type code* consists of 1 to 8 characters where each character must stand for an action, which is to be coupled to this phase. The keyword *TYPE_DEFINITION* on page 18, described below, must be used in the current database to specify what action should be taken by DATA for each character code.

The data entries `[numb. subl.] [sites in subl. 1] [sites in subl. 2]` etc., specify the total number of sublattices (always as an integer digit) and the sites (i.e. stoichiometric coefficients) of each of the sublattices (given in either integer digits or real numerical factors) for the phase.

Optionally, an *auxiliary text string* (maximum 78 characters) can be given after the last [sites in sublattice #] but before the exclamation mark `!`. This string displays in connection with the phase name in some listings within the DATA module.

Examples

```
PHASE GAS:G  % 1 1.0 !
```

```
PHASE LIQUID:L %ZCDQ  2  1.0  1.0
> Metallic liquid solution, modelled by CEF Model. !
PHASE IONIC-LIQ:Y %ZCDQ  2  1.0  1.0
> Ionic liquid solution, modelled by Ionic Two-Sublattice Model. !
PHASE SPINEL:I    %ZA   4   1  2  2  4
> Complex Spinel Solution, by CEF model with ionic constraints. !
PHASE M23C6  % 3 20.0 3.0 6.0 !
PHASE FCC_A1    %&A  2   1 1
> Disordered FCC phase; also as MX carbides/nitrides. !
PHASE FCC_L10   %&AX  3  0.75 0.25 1
> Ordered FCC phase, modelled by 2-Sublattice Model for Ordering. !
PHASE FCC_L12:F %&AX  5  0.25 0.25 0.25 0.25 1.0
> Ordered FCC phase, modelled by 4-Sublattice Model for Ordering. !
PHASE AQUEOUS:A %HIJMR 1 1.0
> Aqueous Solution: using the Complete Revised HKF Model. !
```

CONSTITUENT

```
CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword (and the *ADD_CONSTITUENT* on the next page keyword for large solution phase) defines the phase-constitution as a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase).

The *phase name* (maximum 24 characters) must be a predefined phase (i.e. already through the *PHASE* on page 9 keyword).

It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, SLAG:L, LIQUID:L, IONIC_LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code must also always be attached to the phase name in the CONSTITUENT keyword (and the ADD_CONSTITUENT keyword).

Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent description* (maximum 2000 characters) is a list of the species that enter a phase. The list starts with a colon (`:`), indicating the start of the sub-list of species for the first sublattice, and different sublattices are separated by colons. The complete sequence ends with a final colon.

Optionally, each sublattice may specify which species are considered to be major constituents. This is done by adding a percent sign (`%`) directly to the species name. The start values on the site fractions of the major constituents should sum to 0.99 on a specific sublattice. Thus, the minor constituents (i.e. those without a `%`) add up to 0.01. A maximum of 2000 characters can be coded in the constituent description, continuing in sequent lines. If the phase has a constituent description longer than 2000 characters, the rest can be coded in one or several ADD_CONSTITUENT keywords.

Examples

```
CONSTITUENT BCC_A2 :FE

CONSTITUENT IONIC-LIQ:Y :FE+2 : SB-3: !

CONSTITUENT M23C6 :CR FE :FE CR W MO : C: !

CONSTITUENT AQUEOUS:A :H2O% AG+1 AGF AGCL AGCL2-1 AGI3-2 AGSO4-1
AGC2H4+1

   AGN2H6+1 AGC2N2-1 AGC2H4NO2 AL+3 ALF3 ALO2-1, ... : !

CONSTITUENT SPINEL:I  : AL+3% CR+3 FE+2% FE+3 MG+2% NI+2

                     : AL+3% CA+2 CR+3 FE+2 FE+3 MG+2% NI+2 VA

                     : FE+2 MG+2 VA%

                     : N-3 O-2% :!
```

ADD_CONSTITUENT

```
ADD_CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword adds more constituents to a phase that already has some constituents. Its syntax is the same as for the *CONSTITUENT* on the previous page keyword. This keyword can be used several times, if the phase is very large, e.g. a gaseous mixture or a complex aqueous solution. This is useful when there are so many constituents in a phase that the 2000 characters available for the constituent description list is not enough.

Constituents are not necessary on all sublattices. In the second example below, no addition is made to the first sublattice.

Examples

```
ADD_CONSTITUENT GAS :S1 S2 S3 ... : !

ADD_CONSTITUENT IM-PHASE : :CR:W ... : !

ADD_CONSTITUENT AQUEOUS:A :CUCL+1 CUCL2 CUCL2-1 CUCL3-2 CUOH+1 CUO2H2
CUO3H3-1
```

```
    CUO4H4-2 CU2OH+3 CU2O2H2+2 CU3O4H4+2 NIO2H2 NIO3H3-1 NIO4H4-2
NI2OH+3

    NI4O4H4+4 ZNOH+1 ZNO2H2 ZNO3H3-1 ZNO4H4-2 ... : !
```

COMPOUND_PHASE

```
COMPOUND_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

The keyword is a compact way to simultaneously define a species, a *compound phase* (maximum 24 characters) and its phase-constituent. It is useful for stoichiometric phases with constant compositions. The species name and stoichiometric formula must be identical, i.e. being the given *constituent*. The phase has this species as its only constituent. This keyword allows the database definition file for a large substance database to be more compact; it is a combination of the *SPECIES* on page 8, *PHASE* on page 9 and *CONSTITUENT* on page 14 keywords.

Examples

```
COMPOUND_PHASE AL2O3 % AL2O3 !

COMPOUND_PHASE MAGNETITE %MF FE3O4 !

COMPOUND_PHASE QUARTZ % SIO2 !
```

ALLOTROPIC_PHASE

```
ALLOTROPIC_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

This keyword does the same as the *COMPOUND_PHASE* above keyword for entering an allotropic phase (maximum 24 characters), but does not enter the constituent as a species to the data structure. Use this if the species is already defined.

Examples

```
ALLOTROPIC_PHASE BETHA-AL2O3 % AL2O3 !

ALLOTROPIC_PHASE CRISTOBALITE % SIO2 !

ALLOTROPIC_PHASE TRIDYMITE % SIO2 !
```

TEMPERATURE_LIMITS

```
TEMPERATURE_LIMITS [lower limit] [upper limit] !
```

This keyword sets the default upper and lower temperature limits used by the GIBBS module for Gibbs energy parameters and functions. It can be used only once in one database definition file and all its sequential files.

Example

```
TEMPERATURE_LIMITS 500.0 1800.0 !
```

DEFINE_SYSTEM_DEFAULT

```
DEFINE_SYSTEM_DEFAULT [keyword] {G-ref. type index} !
```

This keyword sets the default value to ELEMENT or SPECIES in the DATA command *DEFINE_SYSTEM* on page 15 in the *Thermo-Calc Console Mode Command Reference*.

For a substance database, it can be appropriate to have ELEMENT as a default value whereas a large solution database can benefit from having SPECIES as a default value. A proper default value is useful for beginners. An advanced user is more likely to use the DATA commands DEFINE_ELEMENT and DEFINE_SPECIES to override the default value.

{G-ref. type index} is an integer indicating the reference state type for an element when entering and listing data in the GIBBS module. The following lists legal numbers and the corresponding meaning (the reference state type for an element):

Number	Definition
1	symbol: G
2	symbol: H298
3	symbol: H0

Example

```
DEFINE_SYSTEM_DEFAULT element 2 !
```

DEFAULT_COMMAND

```
DEFAULT_COMMAND [secondary keyword and parameters] !
```

This keyword specifies commands to be executed by the DATA module at database initialization. The syntax of the available command is currently not the same as the user available DATA commands but the actions are similar. The available *secondary keyword and parameters* in syntax are:

```
DEFINE_SYSTEM_ELEMENT [element names]

DEFINE_SYSTEM_SPECIES [species names]

DEFINE_SYSTEM_CONSTITUENT [phase] [sublattice] [species]

REJECT_SYSTEM_ELEMENT [element names]

REJECT_SYSTEM_SPECIES [species names]

REJECT_SYSTEM_CONSTITUENT [phase] [sublattice] [species]

REJECT_PHASE [phase names]

RESTORE_PHASE [phase names]
```

Examples

```
DEFAULT_COMMAND DEFINE_SYSTEM_ELEMENT FE VA !

DEFAULT_COMMAND REJECT_SYSTEM_CONSTITUENT LIQUID 2 C !
```

```
DEFAULT_COMMAND REJECT_PHASE LIQUID !

DEFAULT_COMMAND RESTOR_PHASE GAS !
```

DATABASE_INFORMATION

```
DATABASE_INFORMATION [text]*10000 !
```

This keyword defines a text for the detailed description of the current database. The text can be listed with the DATA command DATBASE_INFORMATION. An apostrophe (`'`) can be used in the text to indicate a new line; and two apostrophes, (`''`) can be used in the text to indicate a new line plus an empty line.

The continuous *text* length (each line with max 78 characters) is 10,000 characters.

Example

```
DATABASE_INFORMATION This is the XXX-Alloy Solution Database '

      in the A-B-C-D-...... System. '

   Developed by TCS, released in May 2001. ''

... more ... !
```

TYPE_DEFINITION

```
TYPE_DEFINITION [data-type code]*1 [secondary keyword with
parameters] !
```

This keyword couples phases to an action performed by the DATA module when the DATA command *GET_DATA* on page 15 is executed.

Secondary Keywords

The secondary keywords and associated parameters in syntax are:

```
SEQ [filename]

RND# [filename]

GES [valid GIBBS command with parameters]

POLY3 [valid POLY command with parameters]

TDB [valid DATA command with parameters]

IF [conditional statement] THEN [keyword with parameters]

AFTER [valid GIBBS command with parameters]
```

The secondary keyword `SEQ` specifies a sequential file that stores parameters belonging to the phases using the associated data type code (which is defined by this keyword). A special case where the filename is given as an asterisk (`*`) implies that the database definition file also acts as a sequential data storage file. This case makes it possible to have a single file for a small database, which is especially suited for personal databases.

The secondary keyword `RND` should be concatenated with a positive integer `#` to indicate the type of the random file. Currently, there are these types of random files:

- `RND0`, the default, is used for complete Gibbs energy expressions (G0 parameters), where the search field is the unabbreviated parameter name.
- `RND1` is designated for functions, where the function name is used as the search field.
- `RND2` is reserved for binary interaction parameters, where its search field is also the unabbreviated parameter name without any interaction order notation.

Ternary and higher order interaction parameters must be specified on a sequential file. Moreover, the internal structures of these random files are subject to changes with different versions of DATA, and with implementations of DATA on various computer systems. For more information, see the FORTRAN program TDBSORT, which is available from Thermo-Calc Software AB.

The secondary keywords `GES`, `POLY3`, or `TDB` specifies a modification of, or addition to, phases having the associated data type code, such as magnetic contribution, another excess model, or any other valid GIBBS/POLY/DATA command that applies to a certain phase. By implementing this as a call to the interactive GIBBS/POLY/DATA module, flexibility is achieved. If a new type of addition is implemented in a GIBBS/POLY/DATA module, it can be immediately used in the database definition file without reprogramming the DATA module.

In several examples below, the use of the at (`@`) sign indicates any phase to which the relevant type definition (e.g. `A`, `B`, `4`, or `E`) applies.

The secondary keywords `IF` and `THEN` allow specification of a conditional statement structured with respect to the phase constitution that controls the execution of a following type-definition (keyword with parameters) string. See the last four examples.

The secondary keyword `AFTER` is similar to the GES keyword except the defined GIBBS command is executed after all parameters are entered. The reason for this is that the command has no effect unless there is a parameter. Following the `AFTER` keyword, a GIBBS command must be given and it is executed after entering the parameters of the phase.

The data-type code (always as one string) can be any normal or special character, e.g. `0`, `5`, `A`, `F`, `M`, `%`, `&`, and so forth, and is referred in the definition keywords *PHASE* on page 9, *COMPOUND_PHASE* on page 16 and *ALLOTROPIC_PHASE* on page 16 for various phases.

A phase can have several ADDITIONAL parts of different types (that are enforced by certain TYPE_DEFINITIONS which call the GIBBS command AMEND_PHASE_DESCRIPTION for describing various contributions to Gibbs energy). However, the DATA/GIBBS module automatically deletes any early-defined ADDITIONAL part(s) of the same type.

The DATA module can selectively retrieve functions that are necessary for a defined system from a database that has functions stored in its `setup` file or `SEQ` sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces.

Examples

```
TYPE_DEF % SEQ  TCPATH\DATA\[DATABASE]\PARAMETERS.TDB !
TYPE_DEF I SEQ  TCPATH\DATA\[DATABASE]\INTERACTION-PARAMS.TDB !
TYPE_DEF G RND0 TCPATH\DATA\[DATABASE]\GZERO-PARAMS.TDB !
TYPE_DEF F RND1 TCPATH\DATA\[DATABASE]\FUNCTIONS.TDB !
TYPE_DEF & RND2 TCPATH\DATA\[DATABASE]\BINARY-INTERACTIONS.TDB !
TYPE_DEF A GES AM_PH_DES @ MAGNETIC -1 0.40 !
TYPE_DEF B GES AM_PH_DES @ MAGNETIC -3 0.28 !
TYPE_DEF 4 GES AM_PH_DES @ EXCESS_MODEL REDLICH-KISTER_KOHLER !
TYPE_DEF 5 GES AM_PH_DES AQUEOUS EXCESS_MODEL HKF !
TYPE_DEF 6 GES AM_PH_DES AQUEOUS HKF_ELECTROSTATIC !
TYPE_DEF 7 GES AM_PH_DES AQUEOUS STATUS 02084000,,, !
TYPE_DEF 8 GES AM_PH_DES AQUEOUS MAJOR_CONST 1 H2O !
TYPE_DEF E AFTER AM_PH_DES LIQUID EXCESS MIXED-EXCESS
                         A B LEGENDRE   C A POLYNOM ,,,, !
TYPE_DEF T AFTER AM_PH_DES LIQUID TERN-EXT TOOP-KOHLER  B A C ,,,, !
TYPE_DEF Q AFTER AM_PH_DES LIQUID TERN-EXT KOHLER FE CR NI !
TYPE_DEF C IF (PD AND PT AND SN)  THEN TDB RESTORE_PHASE BCT_A5 !
TYPE_DEF D IF (PD AND (PT OR SN)) THEN TDB REJECT_PHASE BCC_A2 !
TYPE_DEF E IF ((NB OR TI OR V) AND (C OR N)) THEN
          GES AM_PH_DES @ COMP_SET ,, CR NB TI V: C N: !
TYPE_DEF F IF (ALO3/2 OR CRO3/2 OR FEO OR MNO OR SIO2) THEN
          GES AM_PH_DES LIQUID COMP_SET ,, ALN%,ALO3/2%,CRO3/2%,
             FEO%,FEO3/2,MNO3/2%,MNS%,SIO2%,TIO2% : !
TYPE_DEF R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS  Fe 0 0.6
         Ag 0 0.01  Al 0 0.05  Ca 0 0.05  Co 0 0.01  Cr 0 0.01
         Cu 0 0.02  Mg 0 0.05  Mn 0 0.05  Mo 0 0.05  Nb 0 0.05
         Ni 0 0.05  Pb 0 0.05  Si 0 0.10  Sn 0 0.02  Ti 0 0.05
         U  0 0.01  V  0 0.02  W  0 0.02  Zr 0 0.03
         B  0 0.01  C  0 0.01  H  0 0.01  N  0 0.01  O  0 0.01
```

```
                  P  0 0.01  S  0 0.01  !
```

Ordered Phase Restores Disorder Contribution

When an ordered phase with disordered contribution is restored, the disordered contribution is automatically restored as well. You can also restore the disordered phase *without* restoring the ordered phase.

However the DIS_PART TYPE_DEFINITION must always be set on the ordered phase. It is important that the disordered phase is declared *before* the ordered phase. Otherwise it causes an error when DIS_PART TYPE_DEFINITION is executed and then either the ordered or disordered phase is rejected.

Example

```
TYPE_DEFINITION & GES A_P_D FCC_A1 MAGNETIC  -3.0    2.80000E-01 !

PHASE FCC_A1  %&  2 1   1 !

    CONSTITUENT FCC_A1  :CR,NI% : C%,VA :  !

$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1

TYPE_DEFINITION ' GES AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_
A1,,,!

TYPE_DEFINITION ( GES A_P_D FCC_L12 MAGNETIC  -3.0    2.80000E-01 !

PHASE FCC_L12  %'(  3 .75   .25   1 !

    CONSTITUENT FCC_L12  :CR,NI% : CR,NI% : C,VA% :  !
```

For example a GES command such as the following only affects phases defined above or at the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( GES A_P_D FCC_L12 DIS_PART FCC_A1,,, !
```

For example a TDB command such as the following only affects phases defined *below* the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( TDB RESTORE_PHASE FCC_A1 !
```

FTP_FILE

```
FTP_FILE [filename] !
```

FTP_FILE is a special function random file and the function names correspond to the record numbers where these record names and the functions are stored. The FTP_FILE decreases search time for the associated database in the DATA module. The file is used for large substance databases along with a SEQ sequential or RND0 random file for storage of G0 parameters referring the functions named `FxxxxT` that are stored in the FTP file. The integer number `xxxx` is a search code used by DATA when such files are processed.

No modification of this file type is allowed.

Example

```
FTP_FILE TCPATH\DATA\[DATABASE]\FTP-FILE.DATA !
```

FUNCTION

```
FUNCTION [function name]*8 [lowest temp. limit]
[expression 2]; [upper temp. limit 2] Y
[expression 1]; [upper temp. limit 1] Y
[expression 3]; [upper temp. limit 2] Y
   .......... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

GIBBS can use predefined functions in the expression (TP-Function) of a Gibbs energy parameter or in other functions. This is often used when several parameters (or functions) have a common sub-expression, such as for metastable modifications of elements. This keyword can appear in both files for database definition and sequential storage, but not in FTP files. A valid *function name* can have up to 8 characters.

A function always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) that are coded as mathematical relations of constants, functions of stable variables (T and P) and other entered functions (normally with a `#` suffix, e.g. `+3*GHSERAL#`).

Also see the *ENTER_PARAMETER* on page 99 in the *Thermo-Calc Console Mode Command Reference*.

The expression is a FORTRAN-like expression and operators `+`, `–`, `*`, `=` and `**` can be used (`**` only with integer powers). Unary-functions `LN` or `LOG` (both for natural logarithm) and `EXP` (for exponential) can also be used. Each expression (TP-Function) should end with a semicolon (`;`), and be followed by its upper applicable temperature limit and a continuation indicator (`Y` to continue with the next expression or `N` to end the function's expression). If there is no continuation after a specific expression (TP-Function), the reference index can optionally be given after the `N` indicator.

A complete/valid function entry can be written in several continuation lines if the function's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.

It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may misunderstand the expression or issue some error messages when reading the function entry. Avoid entering functions like the one below.

```
FUNCTION GHSERXY  298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Such a function is read by the DATA module as

```
1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

rather than

```
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

This is because the DATA module concatenates all lines and removes extra spaces before trying to enter the function in the GIBBS workspace. Thus, the – sign is taken as a delimiter between 298.15 and 1000, and the function incorrectly becomes:

```
FUNCTION GHSERXY 298.15 1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
FUNCTION GHSERXY  298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

which is read correctly as

```
FUNCTION GHSERXY  298.15 -1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a function is normally set by default as 298.15 K, in most cases. However, you can set another limit when it is applicable (according to experimental data and assessments).

An upper-temperature limit (in Kelvin; followed by a `Y` or `N` sign) for the applicability of each TP-Function in a function must be given after the semicolon (`;`) immediately following the specific TP-Function. The highest-temperature limit (in Kelvin) for the applicability of the current function is always followed by the `N` sign. If a negative number is given as the lowest-temperature limit, it assumes there are breakpoints in pressure for this function. In these cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function is also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index *{Ref. Index}* is an integer number indicating where to find the particular function in a special reference file. The references are listed when doing the GET_DATA command in the

DATA module. They can also be listed in the GIBBS module with the command LIST_DATA with the option `R`.

For accounting for the reference indices, also see the keyword *REFERENCE_FILE* on page 35.

The reference index field can also be an abbreviation (such as `REF:250`, `REF_002`, or `REF-SGTE`) which denotes the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option `R`).

However, the references directly coded in the database definition file (`***setup.TDB`) starting with a letter can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option `N` or `R`). Normally, such references must be located after the `LIST_OF_REFERENCE` keyword. It is recommended to use reference code names such as `REF001`, `REF018`, etc. The reference list, which is generated by the GIBBS command *LIST_DATA* on page 77 `<file>` with the `N` or `R` option, is also possible to be directly read by the DATA module.

The DATA module can selectively retrieve functions which are necessary for a defined system from a database that has functions stored in its setup file or SEQ sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces. Previously, this can only be done for large databases that have functions stored in `RND1` random or `FTP` function files.

Examples

```
FUNCTION GFREE  298.15  1000+GFUNXY#; 6000 N !

FUNCTION GFUNXY 298.15 -1000+200*T+30*T*LOG(T); 6000 N 505 !

FUNCTION G0_CAO 298.15 -663538.11+352.67749*T-57.7533*T*LN(T)

        +5.3895E-03*T**2-8.879385E-07*T**3+575530*T**(-1);

     1400.00 Y -625196.99+78.896993*T-20.40145*T*LN(T)

        -1.112923E-02*T**2+5.1896733E-07*T**3-6917350*T**(-1);

     2900.00 Y -499226.55-490.37695*T+51.95912*T*LN(T)

       -2.961051E-02*T**2+1.4033905E-06*T**3-48114685*T**(-1);

     3172.00 Y -587711.89+375.04117-62.76*T*LN(T);

     6000.00 N REF020 !
```

PARAMETER

```
PARAMETER [GIBBS parameter name] [lowest temp. limit]

[expression 1]; [upper temp. limit 1] Y

[expression 2]; [upper temp. limit 2] Y

[expression 3]; [upper temp. limit 2] Y

   .......... ; ..... Y
```

```
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. After the keyword, a valid *GIBBS parameter name* should be given.

It is used to define standard Gibbs energies (i.e. the `G` parameters for Gibbs energy of formations) of all valid end-members of various stoichiometric and solution phases, and excess Gibbs energies (i.e. the `L` parameters for Gibbs energy of interactions) of all binary, ternary, quaternary or higher-order interactions in various solution phases; both standard Gibbs energies and excess energies can also have parameters for contributions from PT-depended volume variations (i.e. the `V0`, `VA`, `VB`, `VC` and `VK` parameters for molar volume, thermal expansivity, bulk modulus, isothermal compressibility and high-pressure fitting parameter), magnetic ordering (i.e. the `TC` and `BM` parameters for Curie temperature and Bohr magneton number) and hypothetical electrostatic interactions (i.e. `BM` parameter for Born functions ωPr,Tr of aqueous solute species).

The general form of a parameter is:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx>
<expression> <yyy> <keyword Y or N> <zzz> !
```

General Form

Name	Description
identifier	The parameter type.
phase	The phase name (maximum 24 characters).
constituent array	The specific constituent array in the phase.
digit	The degree of composition-dependent interaction contribution (an integer number from `0` through `9`), that is only for excess energy (`L`), Curie temperature (`TC`) and Bohr magneton number (`BMAGN`), as well as for volume-related parameters (`V0` or `VA` or `VB` or `VC` or `VK`); if it is valued as zero, or if it is for the standard Gibbs energy (`G`) for which the degree is always zero, it can be omitted.
expression	The mathematical relation to describe the parameter.
xxx and yyy	The low and high temperature limits respectively for the applicable temperature range of the parameter expression
keyword Y or N	The indicator on if there is continuation for the parameter expression or not
zzz	The reference index/number for the assessment of this parameter;
!	The exclamation mark is used to indicate that the current parameter definition is ended

GIBBS Parameter Name

The GIBBS parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Name Examples

Parameter	Definition
`G(GAS,C1O2)`	The Gibbs energy of formation of a CO2 molecule in gas.
`G(FCC,FE:VA)`	The Gibbs energy of formation of fcc Fe with interstitials.
`L(LIQ,Fe,Cr;0)`	The regular solution parameter for Fe and Cr in liquid.
`L(LIQ,Fe,Cr;1)`	The sub-regular solution parameter.
`TC(BCC,Fe:Va)`	The Curie temperature of bcc Fe.
`BMAGN(BCC,Fe:Va)`	The Bohr magneton number parameter of bcc Fe. '

The GIBBS parameter name consists of several parts. The first is a *type-identifier*. The following type-identifiers are legal:

Type-Identifier	**Definition**
G	Standard energy parameter (Gibbs energy of formation)
L	Excess energy parameter (Gibbs energy of interaction)
TC	Curie temperature for magnetic ordering
BMAGN or BM	Bohr magneton number for magnetic ordering (or Born function ωPr,Tr for aqueous solute species).
V0	Molar volume at 298.15 K and 1 bar (a numeric value only)
VA	Integrated thermal expansivity $\int_{298.15}^{T} \alpha(T)dT$
VB	Bulk modulus at 1 bar
VC	Isothermal compressibility
VK	High-pressure fitting parameter

You can also use `G` for interaction parameters; and on output list (performed by the GIBBS command LIST_PARAMETER or LIST_PHASE_DATA) the type-identifier `L` is always used for interaction parameters. Note that the type-identifier `BM` is also used for Born functions ωPr,Tr of aqueous solute species.

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.

It is important that if a phase bears a legal phase-type (among `G`, `A`, `Y`, `L`, `I`, `F` and `B`) in its phase definition (already by the PHASE keyword; such as `GAS:G`, `LIQUID:L`, `SLAG:L`, `IONIC_LIQ:Y`, `SPINEL:I`, `FCC_L12:F`, `HCP_D021:F`, `BCC_B2:B`, `AQUEOUS:A`), such a valid phase-type code should not be attached to the phase name in the PARAMETER keyword.

Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent array* consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents.

Be careful about the sign of odd terms, for example, `L(BCC, B, A:VA;1)` is treated as `L(BCC,A,B:VA;1)`, i.e. it is always put into alphabetical order.

Solution phases with sublattices may have interacting constituents in each sublattice.

You can use an asterisk (`*`) to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L(FCC_L12,AL,NI:*)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the FCC_L12 solution phase, while it is independent of all constituents on the second sublattice. A interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk (`*`) is calculated with the term of [`1-∑y(specified constituents)`], which implies that in an A-B binary system the following three `L` parameters are identical (but in higher-order systems, they are different):

- `L(phase,A,B)` is multiplied with `X(A)*X(B)`
- `L(phase,A,*)` is multiplied with `X(A)*(1-X(A))`
- `L(phase,B,*)` is multiplied with `X(B)*(1-X(B))`

A parameter always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) coded as mathematical relations of constants, functions of stable variables (`T` and `P`) and entered functions (normally with a `#` suffix, e.g. `+3*GSERAL#`).

The expression is a FORTRAN-like expression and operators `+`, `-`, `*`, `=` and `**` can be used (`**` only with integer powers). Unary-functions `LN` or `LOG` (both for natural logarithm) and `EXP` (for exponential) can also be used. Each expression (`TP-Function`) should ends with a semicolon (`;`) and be followed by its upper applicable temperature limit and a continuation indicator (`Y` to continue with the next expression, or `N` to end the parameter's expression). If there is no continuation after a specific expression (TP-Function), the reference index can be optionally given after the `N` indicator.

A complete/valid parameter entry can be written in several continuation lines if the parameter's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.

It is recommended to always have at least one empty space at the beginning of each continuation line. Avoid entering parameters such as:

```
PARAMETR G(LIQUID,A,B) 298.15

-2000+4568*T+2*GFUNAB#; 6000 N !
```

Such a parameter is read by the DATA module as `2000+4568*T+2*GFUNAB#`, rather than as `-2000 +4568*T+2*GFUNAB#`.

Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
PARAMETR G(LIQUID,A,B) 298.15

-2000+4568*T+2*GFUNAB#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a parameter is normally set by default as 298.15 K, in most cases; however, you can set another limit when it is applicable (according to experimental data and assessments). An upper-temperature limit (in Kelvin; followed by a `Y` or `N` sign) for the applicability of each TP-Function in a parameter must be given after the semicolon (`;`) immediately following the specific TP-Function; and the highest-temperature limit (in Kelvin) for the applicability of the current parameter is always followed by the `N` sign. If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this parameter. In such cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current parameter are also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the parameters are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index *{Ref. Index}* is an integer number indicating where to find the particular parameter in a special reference file. The references are listed when doing the GET_DATA command in the DATA module. These can also be listed in the GIBBS module with the command LIST_DATA and the option `R` or `N`.

For accounting the reference indices, also see the keyword *REFERENCE_FILE* on page 35.

The reference index field can also be an abbreviation (such as `REF:250`, `REF_002`, or `REF-SGTE`) denoting the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option `R` or `N`).

However, the references directly coded in the database definition file (`***setup.TDB`) that starts with a letter can be shown when issuing the DATA command `GET_DATA` or the GIBBS command LIST_DATA (with the option `R` or `N`). Normally, such references must be located after the `LIST_OF_REFERENCE` keyword. It is recommended to use reference code names such as `REF001`, `REF018`, etc. The reference list, which is generated by the GIBBS command LIST_DATA `<file>` with the `N` option, is thus also possible to be directly read by the DATA module.

Examples

```
PARAMETER G(BCC,FE:VA) 298.15 1000+200*T+...; 6000 N 91DIN !

PARAMETER TC(BCC,FE:VA)    298.15 +1043; 6000 N 91DIN !

PARAMETER BMAGN(BCC,FE:VA) 298.15 +2.22; 6000 N 91DIN !

PARAMETER G(SIGMA,FE:CR:CR;0) 298.15 1000+200*T+...; 6000 N 101 !

PARAMETER G(LIQUID,AL;0)  298.15  +11005.553-11.840873*T

        +7.9401E-20*T**7+GHSERAL#;

933.60 Y +10481.974-11.252014*T+1.234264E+28*T**(-9)+GHSERAL#;

   2900.00 N  REF:283 !

PARAMETER G(BCC_A2,PB:C)   298.15 UN_ASS#; 300 N REF:0 !

PARAMETER G(BCC_A2,NI:C;0) 298.15 +GHSERNI#+3*GHSERCC#

                                    +400000-100*T; 6000 N REF071 !

PARAMETER G(BCC_A2,MN:VA)  298.15 +GMNBCC#; 6000 N REF285 !

PARAMETER BM(AQUEOUS,OH-1) 298.15 +Z0002PW0#; 1600 N 155 !

PARAMETER L(BCC,FE,CO:VA;0) 298.15 1000+200*T+...; 6000 N !

PARAMETER L(BCC,FE,CO:VA;1) 298.15 1000+200*T+...; 6000 N !

PARAMETER L(BCC,FE,CO:VA;2) 298.15 1000+200*T+...; 6000 N !

PARAM    TC(BCC_A2,CO,MO:VA;0) 298.15  -3700;    6000 N R454 !

PARAM    TC(BCC_A2,CO,MO:VA;1) 298.15  +2300;    6000 N R454 !

PARAM BMAGN(BCC_A2,CO,MO:VA;0) 298.15 -3.445;    6000 N R454 !

PARAM V0(BCC_A2,CR,FE:VA;0) 298.15 +ZERO#; 6000 N REF06V !

PARAM V0(BCC_A2,CR,FE:VA;1) 298.15 -1.10524097E-7; 6000 N REF06V !

PARAM V0(BCC_A2,CR,FE:VA;2) 298.15 +1.40024130E-7; 6000 N REF06V !

PARAM VA(BCC_A2,CR,FE:VA;0) 298.15 -6.49444634E-6*DELTAT#; 6000 N
REF06V !

PARAM VA(BCC_A2,CR,FE:VA;1) 298.15 +2.91269321E-5*DELTAT#; 6000 N
REF06V !
```

OPTIONS

```
OPTIONS /[alloy name]([composition limitations for all alloying
elements]) !
```

This keyword defines an alloy in a database. An alloy has a name, a major component and a number of alloying elements. The purpose for defining an alloy is to be able to tell you about applicable composition limits of the current database in applications to that particular type of alloy. It is possible to have several alloys in the same database. The alloys are given after the keyword in the database.

The alloy name must be proceeded by a slash (`/`) and terminated by the opening parenthesis, with no spaces are allowed in between.

- The alloy name is maximum 8 characters.
- After the parenthesis, follows the major element and a parenthesis with its minimum mass and minimum mole percent given inside.
- Then, the alloying element names, each with its maximum mass and mole percent are given within parenthesis.
- There must a space between definitions for each alloying element.
- The alloy definition is terminated by a closing parenthesis, and the whole OPTIONS keyword by the exclamation mark (`!`).

Example

```
OPTIONS /SSteel(Fe(60,60) CR(30,30) NI(15,15) SI(1,1) N(.1,1)) !
```

TABLE

ⓘ It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may issue some error messages when reading the table entry.

```
TABLE [name]*8 [start temp] [end temp] [delta temp] [table values] !
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. It makes a table of Gibbs energy as a function of temperature where the values are given from the start temperature to the end temperature, at a step of the delta temperature.

Example

```
TABLE DEMTAB 1000.0 1500.0 100.0 -2912.9008 -2834.2416 -2755.5824

                -2677.7600 -2600.7744 -2524.2072 !
```

ASSESSED_SYSTEMS

```
ASSESSED_SYSTEM [descriptions on special treatments for specific
assessed systems]*8000 !
```

This keyword can be included in the database definition file (the `***setup.TDB` file). A maximum of 8000 characters after the keyword (to describe some special options when the DATA, GIBBS and POLY models deal with the existing systems with assessed data) is allowed until the exclamation mark (`!`).

Several ASSESSED_SYSTEMS keywords can be used in the same TDB file in order to have more lists of assessed systems. There is no limit to the number of the entries in the same TDB file.

The assessed systems in the database, and the special treatment options, are typed after the keyword. The elements (always in UPPER CASE) in each assessed system must be in alphabetical order and be separated by a hyphen, such as `C-FE` for the Fe-C binary system, and `C-CR-FE` for the Fe-Cr-C ternary system. A space must be between each assessed system. Information on assessed binary, ternary or higher-order systems may also be given in this way.

A ternary system like C-CR-FE does not imply that the binary C-CR, C-FE and CR-FE are assessed. There is no way to indicate partially assessed systems.

- There is a field to give some descriptive information for a specific system, with various options about how to:
- Reject or restore phase(s) from the current database in the DATA module;
- Set major constituent(s) in the first composition set and to set a second composition set for a specific phase available in the current database in the GIBBS module; *and*
- Calculate this specific system in the POLY module.
- This is the facility used by the BIN (binary phase diagrams) and TERN (ternary phase diagrams) modules in the Thermo-Calc software/database package.

The descriptive information must immediately follow the specific system name, and must be enclosed within parenthesis `(` and `)`, and the left parenthesis must follow directly after the system, such as :

```
AL-NI(TDB +L12 ;G5 C—S:L12/NI:AL:VA ;P3 STP:.8/1200/1 STP:.2/600/1)
```

The syntax TDB means that the commands to the DATA module proceed, and +L12 in the example means that the phase called L12 should be restored (it has been rejected by default).

The directive `;G5` means that the following are commands to the GIBBS module. `C_S:` means creating a second composition set, after the colon follows the phase name and after the slash the major constituents.

After the directive `;P3` follows commands to the POLY module. `STP:` means setting a start point with the value of the X-axis first (composition for the second element in a binary system), the slash separates the Y-axis value (temperature), and possibly one or more directions (`-1`, `1`, `-2` or `2`).

A summary of the allowed syntax is:

TDB accepts

- `+phase` and `-phase` for restore/reject.
- `;G5` accepts
- `MAJ:phase/constituent-array` for major constituents of the first composition set.
- `C_S:phase/constituent-array` for a second composition set.

- `;P3` accepts
- `TMM:lt/ht` for the low-/high-temperature limits (`lt` and `ht`; for instance `TMM:500/4000`) suitable for calculating phase diagrams and property diagrams of a binary system.
- `*` for a default start point which is set as:
- for a binary system: at the composition `X(2`nd `element)=.1234`, temperature `T=1100 K` and with the default directions; or
- for a ternary system: at the compositions `X(2`nd `element)=.1234` and `X(3`rd `element)=.1234` and with the default directions.
- `STP:x/t/d1/d2/d3` for a specific start point in a binary system which is set as at the composition `X(2`nd `element)=x` and temperature `T=t` (in K), and with the directions `d1`, `d2` and/or `d3`.
- `STP:x1/x2/d1/d2/d3` for a specific start point in a ternary system which is set as at the compositions `X(2`nd `element)=x1` and `X(3`rd `element)=x2` and with the directions `d1`, `d2` and/or `d3`.
- The direction(s) can be defined as `-1`, `1`, `-2` or `2`. If no direction is specified, all default directions are used (meaning no `ADD` command is enforced in the POLY module).
- If only one start point is specified, the direction(s) may be omitted; if more than one start points are specified, at least one direction for each start point must be given for all start points.

Each entry for a specific binary or ternary sub-system can be written in one or several lines (each line with 78 characters).

Other Examples

```
ASSESSED_SYSTEMS

AL-NI(TDB +L12 +BCC_B2 ;G5 C_S:L12/NI:AL:VA

       ;P3 STP:.8/1000/1 STP:.45/700/1 STP:.7/700/1)

AL-PB(TDB -HCP -BCC

       ;G5 MAJ:LIQ/AL MAJ:FCC/AL:VA C—S:LIQ/PB C—S:FCC/PB:VA ;P3 *)

CR-FE(;G5 C—S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)

AG-CU(;G5 MAJ:FCC/AG:VA C_S:FCC/CU:VA ;P3 STP:.3/1000)

C-NB(;P3 STP:.9/1100/1)

C-SI(;P3 *)

CO-CR(;G5 MAJ:FCC/CO:VA C_S:FCC/CR:VA ;P3 STP:.1/1100)

CR-FE(TDB -HCP ;G5 C_S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
```

```
CR-NI(;P3 *)

CR-W(;G5 MAJ:BCC/W:VA C_S:BCC/CR:VA

       ;P3 TMM:500/4000 STP:.3/700/1 STP:.3/1800/2 )

CU-FE(TDB -HCP ;G5 MAJ:LIQ/CU MAJ:FCC/FE:VA C_S:FCC/CU:VA

       ;P3 STP:.9/1400)

FE-N(TDB +FE4N ;P3 *)

FE-O(TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:O-2 MAJ:ION_LIQ/FE+2:VA

      ;P3 STP:.2/2000/1 )

FE-S(TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:S MAJ:ION_LIQ/FE+2:S-2
;P3 *)

AL-MG-SI(;P3 *)

C-CR-FE ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA ;P3 *) !
```

The semicolon (`;`) is a part of the `;G5` and `;P3` directives. A long descriptive information can be written in more than one line, such as for the `AL-NI`, `AL-PB`, `CU-FE` and `FE-O` systems shown above.

The directive `;P3 *` is needed if the default start point should be used. If there is no `P3` directive, the BIN or TERN module generates some 20 different start points in order to cover all possible compositions and temperatures (for a binary system) or all possible compositions (for a ternary system under any specific temperature).

REFERENCE_FILE

```
REFERENCE_FILE [file name] !
```

This keyword takes a reference file name as its argument. This reference file (that must be edited in a restrictive way and be saved as a blocked file with a fixed line-length for each line in the file, as described below) contains a complete list of the references for the various parameters (and sometimes functions) in the database. The file must have a fixed record structure: each reference entry with one or several records, and each record with exactly 78 characters written in one single blocked line; and no empty space is allowed at the beginning of all lines in the file. If there are more than one record entered for a reference entry, all the continuation lines must start with an ampersand (`&`). The line number of the first record for a specific reference entry is then accounted as the unique integer for that specific reference, which is referred when a parameter or function calls this integer as the optional *{Ref. Index}*.

Also see keyword *PARAMETER* on page 24 or *FUNCTION* on page 22 about specifying a reference index.

Example

```
/-1<G>            T.C.R.A.S. Class 1
```

```
AG1.64TE1          THERMODATA 01/93

&28/01/93

&SILVER 1.64-TELLURIDE. Solid Standard State.

AG1                HULTGREN SELECTED VAL.        SGTE **

&AT.WEIGHT 107.870,STANDARD STATE:CODATA KEY VALUE.MPT=1234.93K. &--
U.D. 30/10/85.

AG1<G>             T.C.R.A.S  Class: 1

AG1/+1<G>          T.C.R.A.S  Class: 1

AG1BR1             N.P.L.                        SGTE **

&Tfusion uncertain and heat vaporization estimated.

AG1BR1<G>          THERMODATA 01/93

&28/01/93

&Gaseous Standard State.

AG1BR1O3           BARIN & KNACKE.SUPPL.REF:62,* SGTE **

&AGO3BR   SILVER OXYTRIBROMIDE
```

In the example, the unique integers of related references (for assessed elements, species, phases, interactions, etc.) are:

```
1/-1<G>

2AG1.64TE1

5 AG1

8AG1<G>

9AG1/+1<G>

10AG1BR1

12AG1BR1<G>

15AG1BR1O3
```

LIST_OF_REFERENCE

```
LIST_OF_REFERENCE

NUMBER SOURCE

  [REFxxx]  '[Detailed reference]'

..........

.......... !
```

This keyword starts a reference list that is directly coded in the database definition file (`***setup.TDB`). Its argument begins on the following line, and normally has an explanation line (NUMBER SOURCE) that is followed by various reference codes. Each reference code may occupy one or more lines (each line with maximum 78 characters), but must have a reference code name (that starts with a letter) and the detailed reference information (that is written within two single-quotation marks, `''`). It is recommended to use reference code names such as `REF001`, `REF018`, etc. A maximum of 400,000 characters after the keyword is allowed until the exclamation mark (`!`).

Such a reference list can be shown when issuing the DATA command *GET_DATA* on page 15 or the GIBBS command *LIST_DATA* on page 77 (with the `R` option). The reference list, which is generated by the GIBBS command LIST_DATA `<file>` with the `N` option, has this structure, and is thus possible to be directly read by the DATA module.

Example

```
LIST_OF_REFERENCES
NUMBER  SOURCE
REF283 'Alan Dinsdale, SGTE Data for Pure Elements,
          Calphad Vol 15(1991) p 317-425,
          also in NPL Report DMA(A)195 Rev. August 1990'
REF224 'P-Y Chevalier, Thermochimica Acta, 130 (1988) p 33-41; AG-SI'
!
```

ADD_REFERENCE

```
ADD_REFERENCE
  [REFxxx]  '[Detailed reference]'
..........
.......... !
```

Use this keyword to have an unlimited number of references. The use of this is the same as that of *LIST_OF_REFERENCE* on the previous page, and is used after it. Several `ADD_REFERENCES` sections can be used in a single database if there are too many references.

It is recommended to always start with a so-called *empty reference* (such as the `DUMP0` reference in the following example) as the first entry in each of the `ADD_REFERENCE` sections to make sure that all references are listed appropriately as retrieving data by issuing the *GET_DATA* on page 15 command.

Example

```
ADD_REFERENCE
   DUMP0  'Empty reference 0'
   REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
          TRITA 0270 (1986); CR-FE'
   REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
          TRITA 0207 (1986); C-CR-FE'
```

```
   REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys
Database,

          v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters

          at high temperatures.'

   ... ...

!

ADD_REFERENCE

   DUMP1  'Empty reference 1'

   REF275 'A. Fernandez Guillermet, Z. Metallkde. Vol 79(1988) p.524-
536,

          TRITA-MAC 362 (1988); C-CO-NI AND C-CO-FE-NI'

   REF393   'K. Frisk, Metall. Trans. Vol 21A (1990) p 2477-2488,

          TRITA 0409 (1989); CR-FE-N'

   REF1096  'P. Gustafson, Metall. Trans. 19A(1988) p 2547-2554,

          TRITA-MAC 348, (1987); C-CR-FE-W'

   ... ...

!
```

CASE and ENDCASE

```
CASE [ELEMENT/SPECIE/PHASE] !

  IF (boolean algebra on element, species or phase names) THEN

       [GIBBS/POLY/DATA command] !

ENDCASE !
```

This keyword takes as its argument, a definition on which type of the following Boolean algebra operates. A simple Boolean algebra using `AND` and `OR` with a maximum of four levels of parentheses works. The `CASE` construction must end with the `ENDCASE` keyword. This makes it possible to have additional GIBBS or POLY commands executed depending on the user selection of elements, species or phases. The DATA commands that can be given as secondary keyword to *DEFAULT_COMMAND* on page 17 can also be executed.

Example 1

```
CASE ELEMENT !

   IF((CR OR TI OR V) AND N)

   THEN GES AM_PH_DES @ C_S ,, CR MO TI V:C N: !

ENDCASE !
```

Example 2

```
CASE ELEMENT !
```

```
   IF(O) THEN TDB DEFINE_SYSTEM_ELEMENT /- !
ENDCASE !
```

Example 3

```
CASE ELEMENT !
   IF(AL AND FE)
   THEN TDB DEF_SYS_ELEMENT VA !
ENDCASE !
```

VERSION_DATA

```
VERSION_DATE [string]*78 !
```

The string is denoted as the version/revision date and database manager of the database. Nowadays, this directive is used mainly for the purpose of keeping the development and revision history mostly updated.

Example

```
VERSION_DATE Last update and adjustment: Database Manager, 2015-09-25
!
```

Working with the Mobility Databases

In this section:

About the Diffusion Module (DICTRA) and the Databases

A Diffusion Module (DICTRA) installation shares directories with Thermo-Calc, including the `\DATA\` (or `/data/`) area and the database initiation file (`TC_INITD.TDB` or `initd.tdb`).

When you want to switch or add self-generated databases/data-sets or any new database, use the predefined database list in the database initiation file as part of the Thermo-Calc installation packages.

You can add comment lines in the database initiation file, which must start with a $ sign. These lines are ignored by the DATA module. This is also applicable if the database manager or user wants to temporarily disable a database in the predefined database list. If there are too many databases in the \DATA\ area that the DATA module cannot handle properly, the $ sign can be used to temporarily comment about the uncommon databases. However, this does not often happen.

If Thermo-Calc is used with a Windows platform, such additional database initiation files can be located at any directory of any driver, on either a local computer or connected server. The NEW_DICTORY_FILE command displays an **Open** window to access a database initiation file if the file name or its path is not given on the same line of the NEW_DICTORY_FILE command, or if it is incomplete or incorrect, so that the path (in the Look in box) and database initiation file name (in the File name box) can be appropriately selected. However, if Thermo-Calc is run on a Linux/UNIX platform, these files must be located in the current working directory (where Thermo-Calc is started).

In an additional database initiation file, the first database entry may need to have the same path definition structure as in the ordinary database initiation file. Copy the entry line(s) for common databases from the original file to a database initiation file. The entries of the additional databases follow. Similar to the standard databases predefined in the database initiation file, all databases should normally be located in subdirectories under the directory as defined by the `TCPATH` parameter (Windows) or the `TC_DATA` parameter (Linux/UNIX), or under its subdirectory `\DATA\` or `/data/`.

Windows Database Initiation File Example

For a Windows platform, the following example is an additional database initiation file, called `MYINITD1.TDB`:

```
$

$ DATABASES TCC (Additional TCC Databases)

PURE5 TCPATH\DATA\PURE5\PURE5SETU.TDB   SGTE Pure Elements Database,
version 5 !

AD1   TCPATH\DATA\ADD1\AD1SETUP.TDB     TCS ADD1 Solution Database,
version 1 !

AD2   TCPATH\ADDDATA\ADD2\AD2SETUP.TDB  TCS ADD2 Solution Database !

$AD2o  TCPATH\ADDDATA\ADD2old\AD2SETUP.TDB  TCS ADD2 Database (old) !

AD3   TCPATH\DATA\NEWDATA\ADD3\AD3SETUP.TDB  TCS ADD3 Solution
Database !
```

```
AD4    TCPATH\DATA\NEWDATA\MYPROJ1\ADD4\AD4SETUP.TDB
       MYPROJECT1 ADD4 Solution Database !
$
$ DATABASES DIC (Additional DICTRA Databases)
DCAD1 TCPATH\DICDATA\DCADD1\DCAD1SET.TDB
           TCS DCADD1 Mobility Database !
```

Extensions to Database Definition File Syntax

Software packages for simulation of diffusional phase transformations, such as the Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA), need both thermodynamic data and kinetic data (i.e. diffusivities or mobilities). Naturally, the handling and storage of kinetic data also benefits from the use of some kind of database management. Thus, the TDB database definition file syntax has been extended to incorporate some new keywords needed for storing kinetic data - *PARAMETER* on page 24, *DIFFUSION* on the next page, and *ZERO_VOLUME_SPECIES* on the next page.

PARAMETER

```
PARAMETER [special GIBBS parameter name] [low temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
   .......... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

This keyword allows you to enter all types of normal GIBBS parameters for thermodynamic data as well as five special extensions suitable for kinetic data used in the Diffusion Module (DICTRA).

Valid extensions to special GIBBS parameter names are:

- `MQ`: Activation enthalpy for mobility equation.
- `MF`: Pre-exponential factor for mobility equation.
- `DQ`: Activation enthalpy for diffusivity equation.
- `DF`: Pre-exponential factor for diffusivity equation.
- `VS`: Volume counted per mole of volume carrying species.

Examples

```
PARAMETER MQ(BCC,FE:VA) 298.15 1000+200*T+...; 6000 N !
PARAMETER MF(BCC,CO:VA) 298.15 1000+200*T+...; 6000 N !
PARAMETER DQ(FCC,FE:VA) 298.15 1043+...; 6000 N 10 !
```

```
PARAMETER DF(FCC,CR:C ) 298.15 1000+200*T+...; 6000 N 10 !

PARAMETER VS(FCC) 298.15 1000+200*T+...; 6000 N 11 !
```

DIFFUSION

```
DIFFUSION [model keyword] [phase name] [additional parameter(s)] !
```

This keyword specifies the type of diffusion model to use for a phase if the default model is not desired. The default model calculates the full diffusion matrix. A diffusivity is calculated from the different mobilities and the thermodynamic factors. The former ones are calculated as:

```
M = exp (∑MF/RT) exp (∑MQ/RT) / RT
```

where ∑ stands for a weighted summation of the different MF’s and MQ’s plus possibly a Redlich-Kister term.

Valid Model Keywords

Keyword	Description
NONE	No diffusion in this phase
DILUTE	Constitution list of dependent species in each sublattice must be given as an additional parameter. Only the diagonal terms in the diffusion matrix are calculated. D = exp (∑ DF/RT) exp (∑DQ/RT).
SIMPLE	Constitution list of dependent species in each sublattice must be given as additional parameter. Only the diagonal terms in the diffusion matrix are calculated. D = ∑ DF + ∑ DQ.
MAGNETIC	The so-called ALPHA and ALPHA2 parameters must be given as additional parameters. ALPHA is for the substitutional magnetic model and ALPHA2 for the interstitial one. By appending an `&` sign and a species name after the alpha keyword one can supply individual values for the different species. The full diffusion matrix is calculated.

Examples

```
DIFFUSION NONE SIGMA !

DIFFUSION DILUTE CEMENTITE : FE : C : !

DIFFUSION MAGNETIC BCC_A2 ALPHA=0.3 ALPHA2&C=1.8 ALPHA2&N=0.6 !
```

ZERO_VOLUME_SPECIES

```
ZERO_VOLUME_SPECIES [list of species] !
```

In the Diffusion Module (DICTRA), the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes. This keyword uses a list of which species are to be considered as zero volume ones for an argument.

Example

```
ZERO_VOLUME_SPECIES VA C N !
```

Database Definition File Examples

In this section:

Example 1: A Steel Database

```
TEMP-LIM 500.0 2000.0 !

$

$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !

ELEMENT VA VACUUM            0.0     0.0 0.0 !

ELEMENT C  GRAPHITE         12.011   0.0 0.0 !

ELEMENT V  BCC              50.9415  0.0 0.0 !

ELEMENT CR BCC-PARAMAGNETIC 51.996   0.0 0.0 !

ELEMENT FE FCC-PARAMAGNETIC 55.847   0.0 0.0 !

ELEMENT NI FCC-PARAMAGNETIC 58.69    0.0 0.0 !

ELEMENT MO BCC              95.94    0.0 0.0 !

ELEMENT W  BCC             183.85    0.0 0.0 !

$

$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !

PHASE BCC       B1M  2 1.0 3.0 !

PHASE FCC       F2M  2 1.0 1.0 !

PHASE HCP       0    2 2.0 1.0 !

PHASE LIQUID    3    2 1.0 1.0 !

PHASE CEMENTITE 4    2 3.0 1.0 !

PHASE M23C6     4    2 23.0 6.0 !

PHASE M7C3      4    2 7.0 3.0 !

PHASE M6C       4    4 2.0 2.0 2.0 1.0 !

PHASE SIGMA     0    3 10.0 4.0 16.0 !

PHASE MU-PHASE  0    3 7.0 2.0 4.0 !

PHASE R-PHASE   0    3 27.0 14.0 12.0 !

PHASE GRAPHITE  4    1 1.0 !

$

$CONSTITUENT, PHASE-NAME : CONSTITUENTS !

CONSTITUENT BCC :V CR FE NI MO W:VA C: !

CONSTITUENT FCC :V CR FE NI MO W:VA C: !

CONSTITUENT HCP :CR FE NI:VA C N: !

CONSTITUENT LIQUID :C V CR FE NI MO W VA:VA C: !

CONSTITUENT CEMENTITE :CR FE:C: !

CONSTITUENT M23C6 :CR FE:C: !

CONSTITUENT M7C3 :CR FE:C: !

CONSTITUENT M6C :FE:W:FE W:C: !
```

```
CONSTITUENT SIGMA :FE:V CR MO:FE V CR MO: !

CONSTITUENT MU-PHASE :FE:MO W:FE MO W: !

CONSTITUENT R-PHASE :FE:MO :FE MO: !

CONSTITUENT GRAPHITE :C: !

$

$TYPE_DEFINITIIONS:

TYPE-DEFINITION 0 SEQ TCPATH\DATA\METDATA\TC-THEREST.TDB !

TYPE-DEFINITION 1 SEQ TCPATH\DATA\METDATA\TC-BCC.TDB !

TYPE-DEFINITION 2 SEQ TCPATH\DATA\METDATA\TC-FCC.TDB !

TYPE-DEFINITION 3 SEQ TCPATH\DATA\METDATA\TC-LIQUID.TDB !

TYPE-DEFINITION 4 SEQ TCPATH\DATA\METDATA\TC-CARBIDES.TDB !

TYPE-DEFINITION M SEQ TCPATH\DATA\METDATA\TC-CURIE-BOHR.TDB !

TYPE-DEFINITION B GES AM-PH BCC MAGNETIC -1 .4 !

TYPE-DEFINITION F GES AM-PH FCC MAGNETIC -3 .28 !

$

$DEFAULT_COMMANDS:

DEFAULT-COMMAND DEF_ELEMENT VA !

DEFAULT-COMMAND REJ_SYS-CONST LIQUID 1 VA !

$DATABASE_INFORMATION:

DATABASE-INFO The following binary and ternary systems are available: '

  FE-CR-NI by Hertzman'

  FE-MO       Fernandez'

  FE-CR-C     Andersson'

  FE-W-C      Gustafson'

  FE-W        Andersson & Gustafson' !
```

Example 2: A Custom Database for the Sb-Sn Binary System

```
$

$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !

ELEM VA VACUUM             0.0    0.0 0.0 !

ELEM MG HCP(A3)           24.305 0.0 0.0 !

ELEM SB RHOMBOHEDRAL(A7) 121.75   0.0 0.0 !

ELEM SN BCT(A5)          118.69   0.0 0.0 !

ELEM /- ELECTRON-GAS       0      0   0 !

$

$SPECIES, NAME, STOICHIOMETRIC-FORMULA !

SPECIE MG1 MG1!
```

```
SPECIE MG2 MG2!

SPECIE MG2+ MG/+2!

SPECIE SB1 SB1!

SPECIE SB2 SB2!

SPECIE SB4 SB4!

SPECIE SB3- SB/-3!

SPECIE SB5- SB/-5!

SPECIE SN1 SN1!

SPECIE SN4- SN/-4!

$

$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !

PHASE BCT        Z 1 1.0!

PHASE HCP        Z 1 1.0!

PHASE RHOMBO     Z 1 1.0!

PHASE GAS:G      Z 1 1.0!

PHASE LIQUID:L   Z 1 1.0!

PHASE IONICLIQ:Y Z 2 1 1!

PHASE SPLIQ:Y    Z 2 1 1!

PHASE BMG3SB2:I  Z 2 3 2!

PHASE AMG3SB2:I  Z 2 3 2!

PHASE MG2SN:I    Z 2 2 1!

PHASE SBSN       Z 2 1 1!

PHASE SB2SN3     Z 2 2 3!

$

$CONSTITUENT, PHASE-NAME : CONSTITUENTS !

CONSTITUENT RHOMBO :SB SN:!

CONSTITUENT HCP :MG SN:!

CONSTITUENT BCT :SB SN:!

CONSTITUENT GAS:G :MG1 MG2 SB1 SB2 SB4 SN1:

  > Gas phase, using the Ideal EOS and Mixing Model. !

CONSTITUENT LIQUID:L :SB SN:!

CONSTITUENT IONICLIQ:Y :MG2+:SB SB3- SN SN4- VA:

  > This is the Ionic Liquid Solution Phase. !

CONSTITUENT SPLIQ:Y :MG2+:SB SB3- SN SN4- VA:!

CONSTITUENT BMG3SB2:I :MG2+:SB3- SB5- VA SN4-:!

CONSTITUENT AMG3SB2:I :MG2+:SB3- VA SN4-:!
```

```
CONSTITUENT MG2SN:I :MG2+ VA:SB3- SN4-:!

CONSTITUENT SBSN :SB SN:SB SN:!

CONSTITUENT SB2SN3 :SB:SN:!

$

$DEFAULT_COMMANDS:

DEFAULT-COM DEF-ELEM VA /-!

DEFAULT-COM REJ-PHASE LIQUID!

DEFAULT-COM REJ-PHASE SPLIQ!

$

$TYPE_DEFINITIIONS:

TYPE-DEFINITION Z SEQ * !

$

$DATABASE_INFORMATION:

DATABASE_INFO The Sb-Sn system with isentropic temperatures!

$

$VERSION_DATE:

VERSION_DATE Last update 1986-05-18 11:39:49 !

$

$

$ HERE COMES THE THERMODYNAMIC DATA (expressed in functions & parameters):

$

FUNCTION MGLIQUID 298.15 -4630.90976+192.994374*T-34.0888057*T*LOG(T)

   -36544605.6*T**(-2); 6000 N!

$

FUNCTION MGSOLID 298.15 -8367.34+143.677876*T-26.1849785*T*LOG(T)

   +4.858E-4*T**2-1.393669E-6*T**3+78950*T**(-1);

    923.00 Y -13804.4772 +202.909445*T-34.0888057*T*LOG(T)

   -3.65446056E7*T**(-2) +1.06753982E28*T**(-9); 6000 N!

$

FUNCTION SBLIQUID 298.15 9071.98+146.800*T-31.38*T*LOG(T)

   -2.441646E8*T**(-2); 6000 N!

$

.....

..... <more>

$

FUNCTION LFCT 298.15 -17325.6+5.03600*T; 6000 N!
```

```
FUNCTION GFCTSBSN 298.15 LFCT+SBSOLID+SNSOLID+2948.291+3721.286;

   6000 N!

FUNCTION ISB 298.15 15000; 6000 N!

FUNCTION ISN 298.15 47199.9-95.6270*T; 6000 N!

$

.....

..... <more>

$

PARAMETER G(RHOMBO,SB;0) 298.15 SBSOLID; 6000 N!

PARAMETER G(RHOMBO,SN;0) 298.15 2035+SNSOLID; 6000 N!

$

PARAMETER G(HCP,MG;0) 298.15 MGSOLID; 6000 N!

PARAMETER G(HCP,SN;0) 298.15 32000+SNSOLID; 6000 N!

PARAMETER G(HCP,MG,SN;0) 298.15 -69566-9.23183*T; 6000 N!

$

PARAMETER G(BCT,SN;0) 298.15 SNSOLID; 6000 N!

PARAMETER G(BCT,SB;0) 298.15 1000+SBSOLID; 6000 N!

PARAMETER G(BCT,SB,SN;0) 298.15 0.5*ISB+0.5*ISN; 6000 N!

PARAMETER G(BCT,SB,SN;1) 298.15 0.5*ISB-0.5*ISN; 6000 N!

$

PARAMETER G(IONICLIQ,MG2+:SB3-;0) 298.15 -204389-4.98506*T

   -2.75637E9*T**(-2)+3*MGLIQUID+2*SBLIQUID; 6000 N!

PARAMETER G(IONICLIQ,MG2+:SN4-;0) 298.15 -98639.5+881.073*T

   -174.523*T*LOG(T)-1.79808E9*T**(-2); 6000 N!

PARAMETER G(IONICLIQ,MG2+:SB;0) 298.15 SBLIQUID; 6000 N!

$

......

...... <more>

$
```

Example 3: A Public Database for the Fe-Cr-C Ternary System

```
$

$   Revision history:

$       Created as PDEMO  by Pingfang Shi  on 2004-10-05

$       Renamed to DFeCrC by Pingfang Shi  on 2006-10-25

$

$ FURTHER MODIFICATIONS:
```

```
$ ======================
$ pfs: /20041005 (PDEMO)
$       * Retrieved all definitions from PTERN for the Fe-Cr-C ternary !
$
$ pfs: /20061025 (DFeCrC)
$       * Ignore ELEMENT /- definition.
$       * Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$         parameters, in order to avoid BCC-appearance (Fe-C)
$         at temperatures higher than 3900 K.
$           $L(BCC_A2,CR:C,VA;0) 298.15 -190*T;           6000 N REF1 !
$            L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REF1 !
$           $L(BCC_A2,FE:C,VA;0) 298.15 -190*T;           6000 N REF3 !
$            L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REF3 !
$       * Add Cr into HCP_A3 phase, and
$         add all necessary G0/L parameters (according to SSOL2/TCFE3):
$           G(HCP_A3,CR:VA;0)
$           TC(HCP_A3,CR:VA;0)
$           BMAGN(HCP_A3,CR:VA;0)
$           G(HCP_A3,FE:C;0)
$           G(HCP_A3,CR:C;0)
$           L(HCP_A3,CR:C,VA;0)
$           L(HCP_A3,CR,FE:VA;0)
$       * Add "TMM:300/3000" limits to all three binary joins in the
$           ASSESSED_SYSTEM section.
$       * Change the reference indices, e.g., 101 to REF1, in order to
$           always get the reference list correctly.
$       * Re-arrange database format slightly.
$       * Updated the DATABASE_INFO section.
$-------------------------------------------------------------------------
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ DATABASE INFORMATION:
$************************************************************************
$
DATABASE_INFO                                  DFeCrC '
                TCS Demo Fe-Cr-C Alloy Solutions Database'
```

```
         (only for demonstration purposes in TCC-Demo/TCW-Demo)'
      ************************************************************* '
                        (Version 1.2, Oct. 2006) ''
         Copyright @ 2004-2012: Thermo-Calc Software AB, Sweden ''
The DFeCrC database (previously called PDEMO) is the TCS Demo Fe-Cr-C '
Alloy Solutions Database, which is especially designed for primarily '
demonstrating the uses of: '
  * TCC-Demo software: BIN, TERN, SCHEIL and some other modules; '
  * TCW-Demo software: '
     "Binary" module calculations of phase diagrams and property diagrams'
                 in available binary systems; '
     "Ternary" module calculations of phase diagrams (e.g., isothermal'
                 sections, monovariant lines involving liquid, liquidus'
                 surface projections) and property diagrams in available'
                 ternary systems; '
     "Scheil" module simulations of alloy solidifications; and/or '
     "Equilibrium" calculation routines for phase diagrams and property'
                 diagrams in available binary or ternary systems. '
It can also be used for other types of calculations/simulations in both'
TCC and TCW software, and in their application programming interfaces.''
It includes critically-assessed data for all possible three binary joins'
(i.e. Cr-C, Fe-Cr and Fe-Cr) and one complete ternary alloy solutions '
within the Fe-Cr-C system. However, due to the fact that experimental'
data for the Fe-C and Cr-C binary joins and Fe-Cr-C ternary system at '
extremely-high temperatures are not sufficient, the available assessed'
data can not be applied to temperature conditions higher than 4000 K.''
Included thermodynamic data are available for various stoichiometric '
and solution phases, e.g. liquid mixture, various alloy solutions and '
intermetallic phases. But the gaseous mixture phase is excluded in this'
DEMO version.''
The DFeCrC database can be used not only in calculating various types '
of phase diagrams (binary phase diagrams, ternary isothermal sections,'
ternary monovariant lines involving liquid, ternary liquidus surface '
projections, ternary isopleth sections, etc.) and property diagrams '
(the easiest ways are through the BIN and TERN modules), but also in '
simulating alloy solidification processes (with the SCHEIL module) of'
```

```
Fe-based or Cr-based alloys (but limited within the Fe-Cr-C ternary '
system in this DEMO version). Many unique features of the TCC/TCW '
software can be demonstrated using this and other specially-designed '
DEMO databases. ''
However, this DFeCrC database (similar to other DEMO and/or PUBLIC TC '
databases) is provided within the TCC-Demo/TCW-Demo software only for '
the purposes of demonstration, testing and evaluation. For R&D projects'
and teaching activities, you are highly encouraged to only use the FULL'
versions of the TCC and/or TCW software together with some commercial '
databases that are appropriate for your specific applications. Please '
contact us for all kinds of details. ''
Release History: Version 1.1 with minor improvements,  Oct. 2004 '
                 Version 1.2 with minor modifications, Oct. 2006 ''
Edited by: Dr. Pingfang Shi (Thermo-Calc Software, Oct. 2006). ''
!

$ -------------------------------------------------------------------------
$VERSION_DATE Last update and adjustment: Pingfang Shi, 2004-10-05 !
VERSION_DATE Last update and adjustment: Pingfang Shi, 2006-10-25 !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Definition of Elements in the Database System:
$--------------------------------------------------------------------------
$ELEM NAME STABLE_ELEMENT_REF         ATOMIC MASS  H298-H0     S298 !
$--------------------------------------------------------------------------
$ELEMENT /-   ELECTRON_GAS            0.0000E+00  0.0000E+00  0.0000E+00!
ELEMENT VA   VACUUM                  0.0000E+00  0.0000E+00  0.0000E+00!
ELEMENT C    GRAPHITE                1.2011E+01  1.0540E+03  5.7400E+00!
ELEMENT CR   BCC_A2                  5.1996E+01  4.0500E+03  2.3560E+01!
ELEMENT FE   BCC_A2                  5.5847E+01  4.4890E+03  2.7280E+01!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ TYPE_DEFINITIONS for data inclusions:
$--------------------------------------------------------------------------
```

```
TYPE_DEFINITION % SEQ *!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$  TYPE_DEFINITIONS for phase descriptions:
$------------------------------------------------------------------------
$... For magnetic contributions:
TYPE_DEFINITION A GES AMEND_PHASE_DES @ MAGNETIC  -1.0  4.00000E-01 !
TYPE_DEFINITION B GES AMEND_PHASE_DES @ MAGNETIC  -3.0  2.80000E-01 !

$... For Cr/Fe-C in FCC phase and Cr/Fe-C in HCP phase:
TYPE_DEFINITION C IF(C) THEN GES AMEND_PHASE_DES @ C_S ,, :C: !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Default Commands:
$------------------------------------------------------------------------
$DEFINE_SYSTEM_DEFAULT SPECIES 2 !
DEFINE_SYSTEM_DEFAULT ELEMENT 2 !

DEFAULT_COMMAND DEF_SYS_ELEMENT VA !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ FUNCTIONS for various phases:
$------------------------------------------------------------------------
$
FUNCT GHSERCC  298.15 -17368.441+170.73*T-24.3*T*LN(T)
     -4.723E-04*T**2+2562600*T**(-1)-2.643E+08*T**(-2)
     +1.2E+10*T**(-3); 6000 N!
FUNCT GHSERCR  298.15 -8856.94+157.48*T-26.908*T*LN(T)
     +.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);  2180 Y
      -34869.344+344.18*T-50*T*LN(T)-2.88526E+32*T**(-9); 6000 N!
FUNCT GHSERFE  298.15 +1225.7+124.134*T-23.5143*T*LN(T)
     -.00439752*T**2-5.8927E-08*T**3+77359*T**(-1);  1811.00 Y
     -25383.581+299.31255*T-46*T*LN(T)+2.29603E+31*T**(-9); 6000 N!
```

```
FUNCT GFELIQ   298.15 +GHSERFE#+12040.17-6.55843*T
     -3.6751551E-21*T**7;  1811 Y
      -10839.7+291.302*T-46*T*LN(T);  6000 N!
FUNCT GFEFCC   298.15 +GHSERFE#-1462.4+8.282*T
     -1.15*T*LN(T)+6.4E-04*T**2;  1811 Y
      -27098.266+300.25256*T-46*T*LN(T)+2.78854E+31*T**(-9);  6000 N!
FUNCT GFECEM   298.15 +GPCEM1#-10745+706.04*T-120.6*T*LN(T); 6000 N!
FUNCT GFEM23C6  298.15 +7.666667*GFECEM#-1.666667*GHSERCC#
     +66920-40*T; 6000 N!

FUNCT GCRFCC   298.15 +GHSERCR#+7284+.163*T;  6000 N!
FUNCT GCRM23C6 298.15 -521983+3622.24*T-620.965*T*LN(T)
     -.126431*T**2;   6000 N!
FUNCT GCRM3C2  298.15 -100823.8+530.66989*T-89.6694*T*LN(T)
     -.0301188*T**2;  6000 N!
FUNCT GCRM7C3  298.15 -201690+1103.128*T-190.177*T*LN(T)
     -.0578207*T**2;  6000 N!

FUNCT GPCLIQ   298.15 +YCLIQ#*EXP(ZCLIQ#);    6000 N!
FUNCT ACLIQ    298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!
FUNCT BCLIQ    298.15 +1+3.2E-10*P;               6000 N!
FUNCT CCLIQ    298.15 1.6E-10;                    6000 N!
FUNCT DCLIQ    298.15 +1*LN(BCLIQ#);              6000 N!
FUNCT ECLIQ    298.15 +1*LN(CCLIQ#);              6000 N!
FUNCT VCLIQ    298.15 +7.626E-06*EXP(ACLIQ#);     6000 N!
FUNCT XCLIQ    298.15 +1*EXP(.5*DCLIQ#)-1;        6000 N!
FUNCT YCLIQ    298.15 +VCLIQ#*EXP(-ECLIQ#);       6000 N!
FUNCT ZCLIQ    298.15 +1*LN(XCLIQ#);              6000 N!

FUNCT GPCGRA   298.15 +YCGRA#*EXP(ZCGRA#);    6000 N!
FUNCT ACGRA    298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!
FUNCT BCGRA    298.15 +1+3.6E-10*P;               6000 N!
FUNCT CCGRA    298.15 3.3E-10;                    6000 N!
FUNCT DCGRA    298.15 +1*LN(BCGRA#);              6000 N!
FUNCT ECGRA    298.15 +1*LN(CCGRA#);              6000 N!
```

```
FUNCT VCGRA    298.15 +5.259E-06*EXP(ACGRA#);     6000 N!
FUNCT XCGRA    298.15 +1*EXP(.9166667*DCGRA#)-1;  6000 N!
FUNCT YCGRA    298.15 +VCGRA#*EXP(-ECGRA#);       6000 N!
FUNCT ZCGRA    298.15 +1*LN(XCGRA#);              6000 N!

FUNCT GPCFCC   298.15 +YCFCC#*EXP(ZFEFCC#);   6000 N!
FUNCT ACFCC    298.15 +1.44E-04*T;              6000 N!
FUNCT VCFCC    298.15 +1.031E-05*EXP(ACFCC#);   6000 N!
FUNCT YCFCC    298.15 +VCFCC#*EXP(-EFEFCC#);    6000 N!

FUNCT GPCRLIQ  298.15 +YCRLIQ#*EXP(ZCRLIQ#);    6000 N!
FUNCT ACRLIQ   298.15 +1.7E-05*T+9.2E-09*T**2;  6000 N!
FUNCT BCRLIQ   298.15 +1+4.65E-11*P;            6000 N!
FUNCT CCRLIQ   298.15 3.72E-11;                 6000 N!
FUNCT DCRLIQ   298.15 +1*LN(BCRLIQ#);           6000 N!
FUNCT ECRLIQ   298.15 +1*LN(CCRLIQ#);           6000 N!
FUNCT VCRLIQ   298.15 +7.653E-06*EXP(ACRLIQ#);  6000 N!
FUNCT XCRLIQ   298.15 +1*EXP(.8*DCRLIQ#)-1;     6000 N!
FUNCT YCRLIQ   298.15 +VCRLIQ#*EXP(-ECRLIQ#);   6000 N!
FUNCT ZCRLIQ   298.15 +1*LN(XCRLIQ#);           6000 N!

FUNCT GPCRBCC  298.15 +YCRBCC#*EXP(ZCRBCC#);  6000 N!
FUNCT ACRBCC   298.15 +1.7E-05*T+9.2E-09*T**2;  6000 N!
FUNCT BCRBCC   298.15 +1+2.6E-11*P;             6000 N!
FUNCT CCRBCC   298.15 2.08E-11;                 6000 N!
FUNCT DCRBCC   298.15 +1*LN(BCRBCC#);           6000 N!
FUNCT ECRBCC   298.15 +1*LN(CCRBCC#);           6000 N!
FUNCT VCRBCC   298.15 +7.188E-06*EXP(ACRBCC#);  6000 N!
FUNCT XCRBCC   298.15 +1*EXP(.8*DCRBCC#)-1;     6000 N!
FUNCT YCRBCC   298.15 +VCRBCC#*EXP(-ECRBCC#);   6000 N!
FUNCT ZCRBCC   298.15 +1*LN(XCRBCC#);           6000 N!

FUNCT GPFELIQ  298.15 +YFELIQ#*EXP(ZFELIQ#);  6000 N!
FUNCT AFELIQ   298.15 +1.135E-04*T;                           6000 N!
FUNCT BFELIQ   298.15 +1+4.98009787E-12*P+3.20078924E-14*T*P; 6000 N!
FUNCT CFELIQ   298.15 +4.22534787E-12+2.71569924E-14*T;       6000 N!
```

```
FUNCT DFELIQ   298.15 +1*LN(BFELIQ#);                         6000 N!
FUNCT EFELIQ   298.15 +1*LN(CFELIQ#);                         6000 N!
FUNCT VFELIQ   298.15 +6.46677E-06*EXP(AFELIQ#);              6000 N!
FUNCT XFELIQ   298.15 +1*EXP(.8484467*DFELIQ#)-1;             6000 N!
FUNCT YFELIQ   298.15 +VFELIQ#*EXP(-EFELIQ#);                 6000 N!
FUNCT ZFELIQ   298.15 +1*LN(XFELIQ#);                         6000 N!

FUNCT GPFEFCC  298.15 +YFEFCC#*EXP(ZFEFCC#);  6000 N!
FUNCT AFEFCC   298.15 +7.3097E-05*T;                          6000 N!
FUNCT BFEFCC   298.15 +1+3.25236341E-11*P+3.36607808E-16*T*P; 6000 N!
FUNCT CFEFCC   298.15 +2.62285341E-11+2.71455808E-16*T;       6000 N!
FUNCT DFEFCC   298.15 +1*LN(BFEFCC#);                         6000 N!
FUNCT EFEFCC   298.15 +1*LN(CFEFCC#);                         6000 N!
FUNCT VFEFCC   298.15 +6.688726E-06*EXP(AFEFCC#);             6000 N!
FUNCT XFEFCC   298.15 +1*EXP(.8064454*DFEFCC#)-1;             6000 N!
FUNCT YFEFCC   298.15 +VFEFCC#*EXP(-EFEFCC#);                 6000 N!
FUNCT ZFEFCC   298.15 +1*LN(XFEFCC#);                         6000 N!

FUNCT GPFEBCC  298.15 +YFEBCC#*EXP(ZFEBCC#);  6000 N!
FUNCT AFEBCC   298.15 +2.3987E-05*T+1.2845E-08*T**2;          6000 N!
FUNCT BFEBCC   298.15 +1+2.80599565E-11*P+3.06481523E-16*T*P; 6000 N!
FUNCT CFEBCC   298.15 +2.20949565E-11+2.41329523E-16*T;       6000 N!
FUNCT DFEBCC   298.15 +1*LN(BFEBCC#);                         6000 N!
FUNCT EFEBCC   298.15 +1*LN(CFEBCC#);                         6000 N!
FUNCT VFEBCC   298.15 +7.042095E-06*EXP(AFEBCC#);             6000 N!
FUNCT XFEBCC   298.15 +1*EXP(.7874195*DFEBCC#)-1;             6000 N!
FUNCT YFEBCC   298.15 +VFEBCC#*EXP(-EFEBCC#);                 6000 N!
FUNCT ZFEBCC   298.15 +1*LN(XFEBCC#);                         6000 N!

FUNCT GPFEHCP  298.15 +YFEHCP#*EXP(ZFEHCP#);  6000 N!
FUNCT AFEHCP 298.15 +7.3646E-5*T;                           6000 N!
FUNCT BFEHCP 298.15 +1+32.5236341E-12*P+3.36607808E-16*P*T; 6000 N!
FUNCT CFEHCP 298.15 +26.2285341E-12+2.71455808E-16*T;       6000 N!
FUNCT DFEHCP 298.15 +LOG(BFEHCP#);                          6000 N!
FUNCT EFEHCP 298.15 +LOG(CFEHCP#);                          6000 N!
FUNCT VFEHCP 298.15 +6.59121E-6*EXP(AFEHCP#);               6000 N!
```

```
FUNCT XFEHCP 298.15 +EXP(0.8064454*DFEHCP#)-1;              6000 N!

FUNCT YFEHCP 298.15 +VFEHCP#*EXP(-1*EFEHCP#);               6000 N!

FUNCT ZFEHCP 298.15 +LOG(XFEHCP#);                          6000 N!


FUNCT GPCEM1   298.15 +VCEM1#*P;       6000 N!

FUNCT ACEM1    298.15 -1.36E-05*T+4E-08*T**2;      6000 N!

FUNCT VCEM1    298.15 +2.339E-05*EXP(ACEM1#);      6000 N!


FUNCT GPSIG1   298.15 +1.09E-04*P;          6000 N!

FUNCT GPSIG2   298.15 +1.117E-04*P;         6000 N!


$

$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

$ Define the various Phase and their Constituents, and

$ Assign parameters to phases:

$------------------------------------------------------------------------

$PHASE  NAME:TYPE  MARKCODE  #SUBL  SITES_IN_EACH_SUBL. !

$------------------------------------------------------------------------


$***** LIQUID (Solution) ************************************************

PHASE LIQUID:L %  1  1.0

  > This is metallic liquid solution phase, with C species !

CONST LIQUID:L  : C,CR,FE :  !


PARAM G(LIQUID,C;0)  298.15 +GHSERCC#+GPCLIQ#

                               +117369-24.63*T; 6000 N REF0 !

PARAM G(LIQUID,CR;0)  298.15 +GHSERCR#+GPCRLIQ#

                  +24339.955-11.420225*T+2.37615E-21*T**7;  2180 Y

                              +GHSERCR#+GPCRLIQ#

                  +18409.36-8.563683*T+2.88526E+32*T**(-9); 6000 N REF0 !

PARAM G(LIQUID,FE;0)  298.15 +GFELIQ#+GPFELIQ#;  6000 N REF0 !


PARAM L(LIQUID,C,CR;0)  298.15 -90526-25.9116*T; 6000 N REF1 !

PARAM L(LIQUID,C,CR;1)  298.15 +80000;           6000 N REF1 !

PARAM L(LIQUID,C,CR;2)  298.15 +80000;           6000 N REF1 !

PARAM L(LIQUID,C,FE;0)  298.15 -124320+28.5*T;  6000 N REF3 !
```

```
PARAM L(LIQUID,C,FE;1)  298.15  +19300;         6000 N REF3 !

PARAM L(LIQUID,C,FE;2)  298.15  +49260-19*T;    6000 N REF3 !

PARAM L(LIQUID,CR,FE;0)  298.15 -14550+6.65*T;   6000 N REF4 !

PARAM L(LIQUID,C,CR,FE;0)  298.15 -496063;  6000 N REF2 !

PARAM L(LIQUID,C,CR,FE;1)  298.15  +57990;  6000 N REF2 !

PARAM L(LIQUID,C,CR,FE;2)  298.15  +61404;  6000 N REF2 !


$***** FCC_A1 (Solution) ************************************************

$PHASE FCC_A1  %BC  2 1   1 !

$ Note the C TYPE_DEF for 2nd FCC composition-set (MC) is not necessary

$    for the (Fe,Cr)-C system.

PHASE FCC_A1  %B   2 1   1 !

CONST FCC_A1  : CR,FE%

               : C,VA% :  !


PARAM G(FCC_A1,CR:VA;0)  298.15 +GCRFCC#+GPCRBCC#;  6000 N REF0 !

PARAM TC(FCC_A1,CR:VA;0)     298.15 -1109;  6000 N REF0 !

PARAM BMAGN(FCC_A1,CR:VA;0)  298.15 -2.46;  6000 N REF0 !

PARAM G(FCC_A1,FE:VA;0)  298.15 +GFEFCC#+GPFEFCC#;  6000 N REF0 !

PARAM TC(FCC_A1,FE:VA;0)     298.15 -201;  6000 N REF0 !

PARAM BMAGN(FCC_A1,FE:VA;0)  298.15 -2.1;  6000 N REF0 !


PARAM G(FCC_A1,CR:C;0)  298.15 +GHSERCR#+GHSERCC#

                                   +1200-1.94*T;     6000 N REF2 !

PARAM G(FCC_A1,FE:C;0)  298.15 +GFEFCC#+GHSERCC#+GPCFCC#

                                   +77207-15.877*T;  6000 N REF3 !

PARAM TC(FCC_A1,FE:C;0)     298.15 -201;  6000 N REF3 !

PARAM BMAGN(FCC_A1,FE:C;0)  298.15 -2.1;  6000 N REF3 !


PARAM L(FCC_A1,CR:C,VA;0)  298.15 -11977+6.8194*T; 6000 N REF2 !

PARAM L(FCC_A1,FE:C,VA;0)  298.15 -34671;          6000 N REF3 !

PARAM L(FCC_A1,CR,FE:VA;0) 298.15 +10833-7.477*T;  6000 N REF4 !

PARAM L(FCC_A1,CR,FE:VA;1) 298.15  +1410;          6000 N REF4 !

PARAM L(FCC_A1,CR,FE:C;0)  298.15 -74319+3.2353*T; 6000 N REF2 !


$***** BCC_A2 (Solution) ************************************************
```

```
PHASE BCC_A2  %A  2 1   3 !
CONST BCC_A2  : CR%,FE%
              : C,VA% :  !

PARAM G(BCC_A2,CR:VA;0)  298.15 +GHSERCR#+GPCRBCC#;  6000 N REF0 !
PARAM TC(BCC_A2,CR:VA;0)     298.15 -311.5;  6000 N REF0 !
PARAM BMAGN(BCC_A2,CR:VA;0)  298.15   -.01;  6000 N REF0 !
PARAM G(BCC_A2,FE:VA;0)  298.15 +GHSERFE#+GPFEBCC#;  6000 N REF0 !
PARAM TC(BCC_A2,FE:VA;0)     298.15 1043;  6000 N REF0 !
PARAM BMAGN(BCC_A2,FE:VA;0)  298.15 2.22;  6000 N REF0 !

PARAM G(BCC_A2,CR:C;0)  298.15 +GHSERCR#+3*GHSERCC#+GPCRBCC#+3*GPCGRA#
                                  +416000;            6000 N REF1 !
PARAM TC(BCC_A2,CR:C;0)     298.15 -311.5;  6000 N REF1 !
PARAM BMAGN(BCC_A2,CR:C;0)  298.15  -.008;  6000 N REF1 !
PARAM G(BCC_A2,FE:C;0)  298.15 +GHSERFE#+3*GHSERCC#+GPFEBCC#+3*GPCGRA#
                                  +322050+75.667*T;   6000 N REF3 !
PARAM TC(BCC_A2,FE:C;0)     298.15 1043;  6000 N REF3 !
PARAM BMAGN(BCC_A2,FE:C;0)  298.15 2.22;  6000 N REF3 !

$ PF-20061025: Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$         parametera, in order to avoid BCC-appearance (Fe-C)
$         at temperatures higher than 3900 K.
$PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T;           6000 N REF1 !
PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REFS !
$PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T;           6000 N REF3 !
PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REFS !
$
PARAM L(BCC_A2,CR,FE:VA;0) 298.15 +20500-9.68*T;   6000 N REF4 !
PARAM TC(BCC_A2,CR,FE:VA;0)     298.15 1650;  6000 N REF4 !
PARAM TC(BCC_A2,CR,FE:VA;1)     298.15  550;  6000 N REF4 !
PARAM BMAGN(BCC_A2,CR,FE:VA;0)  298.15 -.85;  6000 N REF4 !

PARAM L(BCC_A2,CR,FE:C;0)  298.15 -1250000+667.7*T; 6000 N REF2 !
PARAM TC(BCC_A2,CR,FE:C;0)    298.15 1650;  6000 N REF5 !
PARAM TC(BCC_A2,CR,FE:C;1)    298.15  550;  6000 N REF5 !
```

```
PARAM BMAGN(BCC_A2,CR,FE:C;0) 298.15 -.85;  6000 N REF5 !

$***** HCP_A3 (Solution) ***********************************************
$PHASE HCP_A3  %BC  2 1   .5 !
$ Note the C TYPE_DEF for 2nd HCP composition-set (M2C) is not necessary
$    for the (Fe,Cr)-C system.
PHASE HCP_A3  %B   2 1   .5 !
CONST HCP_A3  : CR,FE,
               : VA%,C :  !

PARAM G(HCP_A3,CR:VA;0) 298.15 +GHSERCR#+4438;           6000 N REF1 !
PARAM TC(HCP_A3,CR:VA;0)    298.15 -1109;  6000 N REF1 !
PARAM BMAGN(HCP_A3,CR:VA;0) 298.15 -2.46;  6000 N REF1 !
PARAM G(HCP_A3,FE:VA;0) 298.15 +GHSERFE#+GPFEHCP#
               -3705.78+12.591*T-1.15*T*LN(T)+6.4E-04*T**2; 1811 Y
                                +GHSERFE#+GPFEHCP#
               -3957.199+5.24951*T+4.9251E+30*T**(-9);      6000 N REF0 !
PARAM G(HCP_A3,CR:C;0) 298.15 +GHSERCR#+.5*GHSERCC#
               -18504+9.4173*T-2.4997*T*LN(T)+.001386*T**2; 6000 N REF1 !
PARAM G(HCP_A3,FE:C;0) 298.15 +GFEFCC#+.5*GHSERCC#+GPCFCC#
                                 +52905-11.9075*T;          6000 N REF3 !

PARAM L(HCP_A3,CR:C,VA;0)  298.15  +4165;  6000 N REF1 !
PARAM L(HCP_A3,FE:C,VA;0)  298.15 -22126;  6000 N REF3 !
$PARAM L(HCP_A3,FE:C,VA;0)  298.15 -17335;  6000 N TCFE3 !
PARAM L(HCP_A3,CR,FE:VA;0) 298.15 +10833-7.477*T; 6000 N REF4 !

$***** SIGMA (Solution) *************************************************
PHASE SIGMA  %  3 8   4   18 !
CONST SIGMA  : FE
              : CR
              : CR,FE :  !

PARAM G(SIGMA,FE:CR:CR;0)  298.15 +8*GFEFCC#+22*GHSERCR#
                                +92300-95.96*T+GPSIG1#;   6000 N REF4 !
PARAM G(SIGMA,FE:CR:FE;0)  298.15 +8*GFEFCC#+4*GHSERCR#+18*GHSERFE#
```

```
                                +117300-95.96*T+GPSIG2#;  6000 N REF4 !

$***** CEMENTITE (Solution) *********************************************
PHASE CEMENTITE  %  2 3   1 !
CONST CEMENTITE  : CR,FE%
                  : C :  !

PARAM G(CEMENTITE,CR:C;0)  298.15 +3*GHSERCR#+GHSERCC#
                                     -48000-9.2888*T; 6000 N REF2 !
PARAM G(CEMENTITE,FE:C;0)  298.15 +GFECEM#;          6000 N REF3 !

PARAM L(CEMENTITE,CR,FE:C;0)  298.15 +25278-17.5*T;  6000 N REF2 !

$***** M3C2 (Compound) **************************************************
PHASE M3C2  %  2 3   2 !
CONST M3C2  : CR
             : C :  !

PARAM G(M3C2,CR:C;0)  298.15 +GCRM3C2#;  6000 N REF2 !

$***** M7C3 (Solution) **************************************************
PHASE M7C3  %  2 7   3 !
CONST M7C3  : CR%,FE
             : C :  !

PARAM G(M7C3,CR:C;0)  298.15 +GCRM7C3#;          6000 N REF2 !
PARAM G(M7C3,FE:C;0)  298.15 +7*GHSERFE#+3*GHSERCC#
                                +75000-48.2168*T; 6000 N REF2 !

PARAM L(M7C3,CR,FE:C;0)  298.15 -4520-10*T;  6000 N REF2 !

$***** M23C6 (Solution) *************************************************
PHASE M23C6  %  3 20   3   6 !
CONST M23C6  : CR%,FE%
              : CR%,FE%
              : C :  !
```

```
PARAM G(M23C6,CR:CR:C;0)  298.15 +GCRM23C6#;           6000 N REF5 !
PARAM G(M23C6,FE:CR:C;0)  298.15 +.1304348*GCRM23C6#
                                   +.8695652*GFEM23C6#; 6000 N REF5 !
PARAM G(M23C6,CR:FE:C;0)  298.15 +.8695652*GCRM23C6#
                                   +.1304348*GFEM23C6#; 6000 N REF5 !
PARAM G(M23C6,FE:FE:C;0)  298.15 +GFEM23C6#;           6000 N REF5 !

PARAM L(M23C6,CR,FE:CR:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !
PARAM L(M23C6,CR,FE:FE:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !

$***** GRAPHITE (Compound) **********************************************
PHASE GRAPHITE  %  1  1.0  !
CONST GRAPHITE  : C :  !

PARAM G(GRAPHITE,C;0)  298.15 +GHSERCC#+GPCGRA#; 6000 N REF0 !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ ASSESSED_SYSTEMS information:
$    *  necessary for the BIN and TERN modules in TCC
$                      the Binary Phase Diagram module in TCW
$                  and the Equilibrium calculation routine in TCW
$------------------------------------------------------------------------
ASSESSED_SYSTEM
$... Binary ...
  C-FE(;P3 TMM:300/4000 *)
  C-CR(;P3 TMM:300/4000 *)
  CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
        ;P3 TMM:300/3000 STP:.6/1200/1/-2/2)
$ CR-FE(TDB -HCP ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
$       ;P3 TMM:300/3000 STP:.6/1200/1/-2/2)
$
$... Ternary ...
  C-CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
          ;P3 STP:.4/.5/1 STP:0.1/0.5/1)
```

```
!


$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$
$ LIST OF REFERENCE:
$
$------------------------------------------------------------------------
LIST_OF_REFERENCES
NUMBER  SOURCE
REF0 'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991)
       p 317-425, also in NPL Report DMA(A)195 Rev. August 1990'
REF1 'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
REF2 'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
REF3 'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267
       TRITA 0237 (1984); C-FE'
REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
       TRITA 0270 (1986); CR-FE'
REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
       TRITA 0207 (1986); C-CR-FE'
REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database,
       v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
       at high temperatures.'
!
```

The Database Checker

In this section:

About the Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.

Thermo-Calc accepts deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and its add-on modules.

The executable **DatabaseChecker** file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu.

Database Checker Revision History below for releases notes that may assist database developers.

Database Checker Revision History

The DatabaseChecker application is standalone and need not be installed separately, just download the containing zip file, open it and follow the instructions in the README.TXT file. The program requires that Java is installed on the target machine. Please note that large amounts of RAM may be required when checking large databases.

Release Notes Version 1.4

- The DatabaseChecker user interface has been modified to allow checking of several database files in one batch. Instead of selecting an individual database file, the user now selects a directory that contains databases. The application then shows a tree structure with all database files in the chosen directory and its subdirectories. The user may then select any number of these files for processing.
- A check of parameters whose interaction order is 3 has been introduced. For such parameters, there must either exist one parameter with the interaction degree 0 or three parameters with the interaction degrees 0, 1 and 2.
- To facilitate optimization of databases, the tool now generates information messages about functions and parameters that will always return 0.

Release Notes, Version 1.3.2

- The tool now detects conflicts between identical parameters even if one of them have been defined with the G prefix and the other with the L prefix.

Release Notes, Version 1.3

A bug prevented integers bigger than 32 bits from being parsed. This has been corrected.

The tool now checks that the species and number of sublattices used in parameter definitions match the phase definition and generates an error message for every mismatch. Ionic liquid parameters are currently exempted from this check as not to break the widespread use of defining only one constituent for ionic liquid parameters.

Type definitions and case statements are now parsed for errors. However, only a subset of all possible GES, POLY and TDB commands are accepted and all other commands will result in an error message. The accepted commands are:

- GES AMEND_PHASE_DESCRIPTION
- COMPOSITION_SETS
- MAJOR_CONSTITUENTS
- DISORDERED_PART
- MAGNETIC_ORDERING
- STATUS_BITS
- DEFAULT_STABLE
- FRACTION_LIMITS
- EXCESS_MODEL

- REDLICH-KISTER_MUGGIANU
- HKF
- HKF_ELECTROSTATIC
- DEBYE_HUCKEL
- GES CHANGE_STATUS
- TDB DEFINE_SYSTEM_ELEMENTS
- TDB RESTORE_PHASES
- TDB REJECT_PHASES

Some improvements to warning and error messages have been made to facilitate finding errors.

Release Notes, Version 1.2

- The tool now uses parallel processing of database files on multi-core systems. This significantly improves performance when large databases are checked.
- It is no longer required that inter-dependent database statements are defined in a specific order in the database file (e.g., species need not any longer be defined before the elements on which they depend). However, for the sake of readability, it is still advised that the database statements occur in a natural order in the file.
- Because of the parallel processing of database statements, multiple definition errors (cases where one name has been used to define more than one entity in the database e.g, two identically named species) may now be generated for any of the violating occurences and not only for the last occurence in the file.

Release Notes, Version 1.1

- Phase names were not properly recognized in parameter definitions if there was one or more whitespace characters between the opening parenthesis and the phase name. This has been corrected.
- The error message Could not parse parameter, <species name> has been given without a sublattice number but is defined in more than one sublattice is now displayed only for phases where the general diffusion model is used. Note: this implementation is temporary and may be subject to changes later.
- The meaning of the information message The phase <phase name> expects the following parameters: [<parameter names>] was unclear to users. It is now longer shown for the parameter names T and P. For all other names, the message is now displayed as an error message with the following text: The phase <phase name> contains references to the following undefined functions: [<function names>].

- The tool now looks for function names that are abbreviations of other function names and warns about this, since abbreviated names may cause problems during the execution of macro files that have been auto-generated from GES.
- The tools also warns for functions whose names are in the format V<integer>, since this may cause conflicts with names that are used by PARROT.
- Parameter names are now shown in a format that is less cryptic and more resembles the format used in the database. However, the format of diffusion parameters may still differ somewhat from what is used in the database.

Release Notes, Version 1.0

- The tool parses a TDB file and produces a log with error, warning and information messages about the state of the file
- The message log can be exported and saved as a separate file for later analysis
- The tool is based on the database command definitions given in TC_Database_ManagersGuide and DICTRA27_UsersGuide. All commands in these documents are supported. Some undocumented DIFFUSION commands are not supported.
- Databases that span several files are correctly handled, also blocked files
- The tool is in some aspects more strict than required by the guides (see Additional Information below)
- The tool performs the following checks:
- Syntax control of database statements: ERROR
- Line size: ERROR or WARNING depending on context
- Multiply defined elements, species or phases: ERROR
- Multiply defined functions and parameters: ERROR
- Multiply defined assessed system: ERROR
- Multiply defined references: ERROR
- References entries that are never used: WARNING
- References to non-existent type definitions: ERROR
- Type definitions that are never used: WARNING
- Unused functions and parameters: WARNING
- Functions and parameters with undefined references: WARNING
- References to undefined elements, species or phases: ERROR

- Dependencies to external names from a phase: INFORMATION. (All parameters of a phase are evaluated with respect to their dependencies to other parameters and functions and all unresolved names are listed. Typically, this should only yield dependencies on T and possibly P)

Additional Information

In addition to the command definitions given in the user guides listed above, the following rules are also applied:

- Names are case-sensitive, meaning that e.g., the defined element MN cannot be referred to under the name Mn;
- Phase names cannot be abbreviated. When referred to in parameter descriptions their full names must be used.

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