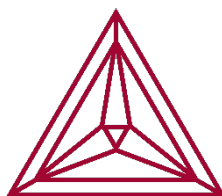




Console Mode Command Reference

Thermo-Calc Version 2015b



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2. About the Console Command Reference

This command reference is for Console Mode users of the Thermo-Calc program. This guide describes the function and syntax of the commands available in the Thermo-Calc modules. It is also useful for DICTRA users, although the specific DICTRA commands are described in the *DICTRA Command Reference*, which can be found either by searching the online help or on the [Thermo-Calc website](#).

The commands available in all or most modules are described in the first section ([General Commands](#)). The next sections are listed in alphabetical order based on the module names, then in each subsection, the module commands.

- [Typographical Conventions](#)
- [Help Resources](#)
- [File Types](#)

2.1 Typographical Conventions

The following conventions are used throughout the documentation:

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 .
<i>Italic</i> font	An <i>italic</i> font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
COMMAND	This font and all capital letters indicates that this is a COMMAND used in the Console Mode terminal.
Hyperlink	Text in blue and underline is a link to another section. In this document commands are also sections. Clicking this link will take you to more detail about a particular command.
PROMPT	The ALL CAPS CODE FONT indicates this is a prompt on the terminal asking for input or an option presented on the terminal after a COMMAND is entered.
<Enter>	Text with <angle brackets> indicates a keyboard entry. Usually to press Enter (or Return).
SYNTAX	ALL CAPITALS indicates this is the command category, the command that is entered in the Console Mode. Information about the command follow.
code and code bold	A code font shows a programming code or code example. The code bold font highlights the entry.


2.1.1 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`.

2.2 Help Resources

Online Help

- To access online help, open Thermo-Calc and select **Help→Online Help**.
- To access some feature help in Graphical Mode, in the lower left corner of the Configuration window, click the help button  for information about the active tab or node.


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.

PDFs

- On [Thermo-Calc Software's website](#).
- Wherever the software is installed, folders containing the PDFs versions of the documentation are also downloaded. See the *Thermo-Calc Installation Guide* for details of where these are installed for your operating system.

Examples

 On a Windows network user login, the Thermo-Calc and DICTRA Examples and Materials folders are installed here **C:\Users\Public\Documents\Thermo-Calc\2015b**. The TC_PRISMA Examples folder is installed here **C:\Users\<user>\Documents\Thermo-Calc\2015b**. For all products, the manuals are installed here **C:\Program Files\Thermo-Calc\2015b\Manuals**.

 On Windows, once Thermo-Calc is installed, you can also locate the Thermo-Calc and DICTRA Examples and Materials folders, plus all the Manuals using the shortcuts located in the Start menu. Go to **Start → All Programs >Thermo-Calc** and click **Examples**, **Manuals**, or **Materials** as required to open the applicable folder. The TC_PRISMA Examples folder is currently available from here **C:\Users\<user>\Documents\Thermo-Calc\2015b**.

See the *Thermo-Calc Installation Guide* for details for other operating systems to learn where these are installed.

2.3 File Types

Also refer to the *Thermo-Calc Installation Guide* for database default directories.

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) (see the *Data Optimisation User Guide* for information).
- The GIBBS module uses a workspace file (*.GES5)
- The PARROT module uses files with the suffixes *.PAR and *.POP.

3. General Commands

- [BACK](#)
- [EXIT](#)
- [GOTO_MODULE](#)
- [HELP \(? and ??\)](#)
- [HELP](#)
- [INFORMATION](#)
- [MACRO_FILE_OPEN](#)
- [SET_INTERACTIVE](#)

3.1 BACK

Switch control back to the most recent module. See also the GOTO_MODULE command. Going from the POST module (post-processor), back goes only to the TAB or POLY module (from where the POST module is entered).

Syntax	BACK
--------	------

3.2 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).

Syntax	EXIT
--------	------

3.3 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>
Options	<p>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</p> <pre> 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: </pre>

3.4 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). For some commands and prompts, more detailed help is given when two ?? are entered.

Syntax	? OR ??
--------	---------

3.5 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	<p>COMMAND: <COMMAND NAME></p> <p><i>Command name</i> is the name of the command (one of the-module commands) to get help.</p> <p>If the <Enter> key is pressed without typing a command name, then all the available commands are listed.</p>

3.6 INFORMATION

Get basic information about topics related to the module you are in.

Syntax	INFORMATION
Prompt	<p>WHICH SUBJECT /PURPOSE/: <TOPIC NAME></p> <p>Specify a Subject (or its abbreviation as long as it is unique). Enter a question mark ? for a list of topics.</p>

3.7 MACRO_FILE_OPEN

The macro file functionality is a way to predefine sequences of Thermo-Calc (and DICTRA) 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) 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).



See the [Thermo-Calc User Guide](#) on the website as well as Example 12 in the *Console Mode Examples*.

This is useful when the same/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](#) 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 Console Mode (and DICTRA) program.

All Thermo-Calc and DICTRA 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 [SET INTERACTIVE MODE](#) 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](#) 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 Thermo-Calc (Console Mode) (and DICTRA) software, all enforced according to the macro file(s).

3.7.1 Prompts and Options

Syntax	MACRO_FILE_OPEN
Prompt	<p><name of a macro file *.tcm></p> <p>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.</p>

	<p>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.</p> <p>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.</p> <p>When using a macro file that intended to plot graphs on screen, but the command SET_PLOT_FORMAT 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.</p> <p> For an extensive example about using macro features for the TAB-Module, see examples file 12 in the Thermo-Calc Console Mode Examples.</p>
--	--

3.8 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.

Syntax	SET_INTERACTIVE
--------	-----------------

4. DATABASE_RETRIEVAL Commands

- [AMEND_SELECTION](#)
- [APPEND_DATABASE](#)
- [DATABASE_INFORMATION](#)
- [DEFINE_ELEMENTS](#)
- [DEFINE_SPECIES](#)
- [DEFINE_SYSTEM](#)
- [GET_DATA](#)
- [LIST_DATABASE](#)
- [LIST_SYSTEM](#)
- [NEW_DIRECTORY_FILE](#)
- [REJECT](#)
- [RESTORE](#)
- [SET_AUTO_APPEND_DATABASE](#)
- [SWITCH_DATABASE](#)



Search the online help or see the [Thermo-Calc User Guide](#) on the website for step-by-step instructions to define a system.

4.1 AMEND_SELECTION

Use this after defining the elements, species or the system (with the commands [DEFINE_ELEMENTS](#), [DEFINE_SPECIES](#), or [DEFINE_SYSTEM](#)). 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

4.2 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 the [SWITCH_DATABASE](#) command, 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 the [NEW DIRECTORY FILE](#) command, 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	<p>Use one of these databases</p> <pre>PURE = SGTE PURE ELEMENT DATABASE SSUB = SGTE SUBSTANCE DATABASE 1997 USER = USER DEFINED DATABASE DATABASE NAME /XYZ/: <ADDITIONAL DATABASE NAME></pre>
Options	<p>ADDITIONAL DATABASE NAME</p> <p>The name of an existing database or a USER database definition file (<code>***setup.TDB</code>) that corresponds to the appending database.</p>

APPEND_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.

4.3 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.

Syntax	DATABASE_INFORMATION
--------	----------------------

4.4 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 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 the [DEFINE_SPECIES](#) or [DEFINE_SYSTEM](#) commands must be repeated with the same or similar elements as defined in the first switched database.

4.5 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 the *Thermo-Calc User Guide* for step-by-step instructions to define a system with this command.

Syntax	DEFINE_SPECIES
Prompt	SPECIES& <SPECIES1, SPECIES2, ...> A list of species to be defined in the system.

When appending database(s), this command, the [DEFINE_ELEMENTS](#) or [DEFINE_SYSTEM](#) commands must be repeated with the same or similar elements as defined in the first switched database.

4.6 DEFINE_SYSTEM

Define the system in terms of either elements (equivalent to [DEFINE_ELEMENTS](#)) or species (equivalent to [DEFINE_SPECIES](#)). 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 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, ...>
<i>Options</i>	<i>Description</i>
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.

4.7 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.



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
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4.8 LIST_DATABASE

List all elements, species, phases or phase constituents in the database.

Syntax	LIST_DATABASE
<i>Options</i>	<i>Description</i>
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.

4.9 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 the LIST_DATABASE command) must be used to indicate what to list.

4.10 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.

 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.

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.

4.11 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](#)). 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)

	<p>PHASE: <PHASE NAME></p> <p>SUBLATTICE NUMBER: <SUBLATTICE NUMBER IN THE PHASE></p> <p>CONSTITUENT: <CONSTITUENT(S) IN THE SUBLATTICE OF THE PHASE></p>
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	<p>The given constituent in one phase are rejected. Add the following when prompted:</p> <p>Phase: The name of the phase containing the constituent to be rejected.</p> <p>Sublattice number: The sublattice where the constituent enters (the first sublattice is 1). The question is omitted if there exists only one possible sublattice.</p> <p>Constituent: The name(s) of the constituent(s) to be rejected.</p>

4.12 RESTORE

Restore already explicitly rejected elements, species, phases or constituents; it is the opposite of the command REJECT 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](#)). 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
Prompt 1	(if keyword = ELEMENTS or SPECIES or PHASES) 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>
Options	Description and Additional 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.

4.13 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](#) or [APPEND_DATABASE](#)). This is useful to simultaneously retrieve both thermodynamic and mobility data for a defined system when performing a DICTRA simulation.

This command should be used before defining a system (with the commands [DEFINE_ELEMENTS](#), [DEFINE_SPECIES](#), or [DEFINE_SYSTEM](#)) and retrieving the data with the [GET_DATA](#) command from the primary switched 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 the GET_DATA command afterwards.

Syntax 1	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.

4.14 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 the [NEW_DIRECTORY_FILE](#) command, 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	Use one of these databases: <ul style="list-style-type: none"> • PURE (SGTE pure element database) • SSUB (SGTE substance database 1997) • USER (user-defined database) DATABASE NAME /XYZ/: <NEW DATABASE NAME>

Options	Description and additional information
NEW DATABASE NAME	The name of an existing database or a USER database definition file (**setup.TDB).
DATABASE NAME	<p>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 from Thermo-Calc Software or its agents, you can add these to the predefined database list in the database initiation file TC_INITD.TDB or initd.tdb of your installed Thermo-Calc/DICTRA packages.</p> <p>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.</p>
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.

SWITCH_DATABASE 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.

5. 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. Read [Running the EDIT_EXPERIMENTS Command](#) section before beginning.

- [COMPUTE_ALL_EQUILIBRIA](#)
- [EXPERIMENT](#)
- [EXPORT](#)
- [IMPORT](#)
- [LABEL_DATA](#)
- [LIST_ALL_EQUILIBRIA](#)
- [MAKE_POP_FILE](#)
- [READ \(READ_WORKSPACE = READ_BLOCK\)](#)
- [RESTORE_ALL_WEIGHTS](#)
- [SAVE_WORKSPACES](#)
- [SET_ALTERNATE_CONDITION](#)
- [SET_WEIGHT](#)
- [STORE_ALL_WEIGHTS](#)
- [TRANSFER_START_VALUE](#)

5.1 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 the [EDIT_EXPERIMENTS](#) command in the PARROT module) should always be the read (READ_BLOCK) command, 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 give a SAVE-WORKSPACE command 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.

5.2 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 the CREATE_NEW_EQUILIBRIUM command, and stored in an experimental data *.POP file and then compiled and saved in the POLY3 workspace of a PARROT work *.PAR file.

Syntax	COMPUTE_ALL_EQUILIBRIA
--------	------------------------

With the COMPUTE-ALL-EQUILIBRIA command, 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 the [SELECT EQUILIBRIUM](#) command so that the current point is switched to a desired one.


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 by the [LABEL DATA](#) command, 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 command 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).

5.3 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: the first one as a quantity relation, and the second one as the uncertainty of the value for the quantity, with a colon (:) separating them. The quantity relation part 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
	<p>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, <code>T=1273.15:5</code>. An inequality, < or >, can also be used. For example:</p> <p><code>ACR(C) < -0.01:0.001, W(BCC, AG) > 0.05:10%</code></p>

Important note

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 a [SET_REFERENCE_STATE](#) command. 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
```

5.4 EXPORT

Transfer/export a calculated value from an equilibrium to an optimising 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	<p>FUNCTION NAME: <FUNCTION NAME>#<N></p> <p>Specify the name of the function, the value of which should be transferred to a ∇ variable. The number (n) of the ∇ variable must be given after the function name, separated by hash character #.</p>

Important note	<p>The function name is UPPER/lowercase sensitive, and it should normally be given in UPPER case. For example,</p> <pre>ENTER_FUNCTION STRNGY=GM(FCC) .X(CU) ;</pre> <pre>EXPORT STRNGY#6</pre> <p>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. v_6).</p>
----------------	--

5.5 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 the [EXPORT](#) command.


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.



Another case when this command is useful is shown in the *.POP file of Example 36 as given in the /TCEX/ subdirectory of a Thermo-Calc installation and described in [Thermo-Calc Console Mode Examples](#) files you can download from the website.

Syntax	IMPORT
Prompt	<p>CONSTANT NAME: <CONSTANT NAME>#<N></p> <p>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 #.</p> <p> The constant name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.</p> <p>For example:</p> <pre>ENTER_CONSTANT ACU=0.1</pre> <pre>IMPORT ACU#2</pre> <p>This transfers the value of the optimizing variable 2 (i.e. v_2) to the constant ACU.</p>

5.6 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 [SET WEIGHT](#) command to assign the same weight to all equilibria with the same label.

Syntax	LABEL_DATA
Prompt	<p>LABEL? /A1/: A<BCD></p> <p>Specify a textual label (as maximum characters and must start with the letter A) for the current experimental equilibrium point(s).</p>

5.7 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 the [SELECT EQUILIBRIUM](#) command to select a specific point as the current equilibrium point for such a list.


Syntax	LIST_ALL_EQUILIBRIA
--------	---------------------

5.8 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 DICTRA, an *.DOP file is written or overwritten.

Syntax	MAKE_POP_FILE
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <POP/DOP-FILE NAME></p> <p>Specify a name of the new *.POP/*.DOP file where to write or overwrite the edited experimental information in a simple text format.</p>

5.9 READ (READ_WORKSPACE = READ_BLOCK)

This command (previously named read-block) is equivalent to the read-workspaces command in the POLY module, but it only reads the POLY3 workspace from the work file set by the [SET_STORE_FILE](#) command in the PARROT module.

Syntax	READ
Prompt	BLOCK NUMBER /#/ : <N> The number of data block that should be edited must be given. If there is no FLUSH_BUFFER command in the original POP or DOP file, then there is only one data block with the number 1.

 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 any [LIST_RESULT](#) or [OPTIMIZE_VARIABLES](#) command in PARROT in between.

5.10 RESTORE_ALL_WEIGHTS

Restore a specific weight-set (previously saved by the [STORE_ALL_WEIGHTS](#) command) 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.

5.11 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 the [SAVE_PARROT_WORKSPACES](#) command 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 the OPTIMIZE_VARIABLES command the computed results are automatically updated.

Syntax	SAVE_WORKSPACES
Prompt	<FILE NAME> <Y OR N>


 Sometimes good starting values (SET_START_VALUE) 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.

5.12 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 while the uncertainty should also be specified.

Syntax	SET_ALTERNATE_CONDITION
--------	-------------------------

 The alternate condition (including the normally POLY-module condition plus uncertainty; 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.

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 additional information
State variables	<p>Some of the state variables that can be used in conditions are:</p> <ul style="list-style-type: none"> • 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)

Options	Description and additional information
	<ul style="list-style-type: none"> HM (<phase>) (enthalpy of a phase per mole)
Additional prompts	<p>FACTOR: <A FACTOR FOR THE STATE VARIABLE, OR A CONTINUATION></p> <p>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:</p> $2 * \text{MUR}(\text{FE}) + 3 * \text{MUR}(\text{O}) = -35000$ <p>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.</p>
	<p>STATE VARIABLE: <A SPECIFIED STATE VARIABLE, OR A CONTINUATION></p> <p>This question is prompted if a single state variable name has not given in either the prompt <code>State variable expression</code> or <code>Factor</code>, or a state variable expression is given but the expression is incomplete, for example, <code>T-</code> or <code>2*MUR(FE)+</code>, 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).</p>
	<p>VALUE /X/: <A NUMERIC VALUE, A CONSTANT OR A VARIABLE></p> <p>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 <code>NONE</code> means that the condition is removed.</p>
	<p>UNCERTAINTY /NONE/: <UNCERTAINTY OF THE CONDITION></p> <p>The uncertainty of the condition. This can be a numeric value, a constant or a variable. The default value <code>NONE</code> 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 (<code>x%</code>).</p>

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:

$$X(\text{LIQ}, S) - X(\text{PYRR}, S) = 0$$

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.


5.13 SET_WEIGHT



Each experimental value has an uncertainty associated with it, specified by the value after the colon (:) in the [EXPERIMENT](#) command. 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 the COMPUTE_ALL_EQUILIBRIA command is given) and in OPTIMIZATION 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	<p>VALUE /1/: <WEIGHT VALUE></p> <p>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.</p> <p> 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.</p>
	EQUILIBRIA (RANGE) OR LABEL(S) /PRESENT/: <SELECTION>

	<p>Define the equilibria. These are available in the read data block from the current work file and are given the above-defined weight.</p> <p>The selection may be given as a range but the equilibrium numbers must then be separated only by a minus sign.</p> <p> The start and end equilibrium numbers must be available in the read data block read from the current work file.</p> <p>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.</p> <p>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.</p> <p>By pressing <Enter> to accept the default value <code>present</code>, the above defined weight is only assigned to the current or present experimental point (which is selected by the POLY command SELECT EQUILIBRIUM).</p> <p> If a <code>COMPUTE_ALL_EQUILIBRIUM</code> command is used but no specific equilibrium point is selected afterwards, the last point in the read data block remains the <code>present</code> point.</p>
--	--

5.14 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 by the [RESTORE_ALL_WEIGHTS](#) command sequentially.

Syntax	STORE_ALL_WEIGHTS
Prompt	<p>COMMAND LINE: <WEIGHT-SET NAME></p> <p>Give a weight-set name (comment line texts) for the current weight set for all experimental points.</p>

5.15 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	<p>FROM EQUILIBRIUM /PREVIOUS/: <EQUILIBRIUM NUMBER></p> <p>The equilibrium number is the numeric identifier for the equilibrium from which the start values should be copied to the present experimental point. <i>Previous</i> is the default if you press <Enter>.</p>

6. Experimental Data Files

- [Commands in the Experimental Data Files \(*.POP, *.DOP\)](#)
- [TABLE HEAD, TABLE VALUES and TABLE END](#)
- [COMMENT](#)
- [FLUSH BUFFER](#)

6.1 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, and can thus be used by Thermo-Calc or DICTRA in any CPU platform.


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_EXPERIMENT 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.


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
- CHANGE_STATUS
- SET_CONDITION
- SET_REFERENCE_STATE
- ENTER_SYMBOL
- SAVE_WORKSPACE

 As the last command in an *.POP or *.DOP file, you must always have the SAVE command.

Other legal commands from the POLY module that are used less often are:

- DEFINE-COMPONENTS
- EVALUATE-FUNCTION
- SET-ALL-START-VALUES
- SET-NUMERICAL-LIMITS
- SET-START-VALUE
- ADVANCED-OPTIONS

 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
- EXPORT
- IMPORT
- LABEL-DATA
- SET-ALTERNATE-CONDITION
- SET-WEIGHT

However, 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 the Thermo-Calc/DICTRA software family, 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.

6.2 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.

Prompts and Options

Syntax	TABLE_HEAD
	TABLE_VALUES
	TABLE_END

Notes

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.

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. 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

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 at the CREATE-NEW-EQUILIBRIUM command. 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.

6.3 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. A comment can have a maximum of about 60 characters written on the same line.

Syntax	COMMENT
--------	---------

6.4 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 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.

After a FLUSH 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.

Syntax	FLUSH_BUFFER
--------	--------------

7. GIBBS_ENERGY_SYSTEM Commands

- [ADD_COMMENT](#)
- [AMEND_ELEMENT_DATA](#)
- [AMEND_PARAMETER](#)
- [AMEND_PHASE_DESCRIPTION](#)
- [AMEND_SYMBOL](#)
- [CHANGE_STATUS](#)
- [ENTER_ELEMENT](#)
- [ENTER_PARAMETER](#)
- [ENTER_PHASE](#)
- [ENTER_SPECIES](#)
- [ENTER_SYMBOL](#)
- [LIST_CONSTITUENT](#)
- [LIST_DATA](#)
- [LIST_PARAMETER](#)
- [LIST_PHASE_DATA](#)
- [LIST_STATUS](#)
- [LIST_SYMBOL](#)
- [READ_GES_WORKSPACE](#)
- [REINITIATE](#)
- [SAVE_GES_WORKSPACE](#)
- [SET_R_AND_P_NORM](#)

7.1 ADD_COMMENT


Add a comment or make notes about parameters and so forth.

Syntax ADD_COMMENT

7.2 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	<p>ELEMENT NAME: <ELEMENT NAME></p> <p>Specify the name of the element for which you want to change the data.</p>
	<p>NEW STABLE ELEMENT REFERENCE /ABCD/: <NAME OF SER></p>

	<p>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.</p>
	<p>NEW ATOMIC MASS /XX.XXXX/: <YYYYYY></p> <p>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.</p>
	<p>NEW H(298.15)-H(0) /XXX.XXX/: <YYYYYY></p> <p>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.</p>
	<p>NEW S(298.15) /XX.XXXX/: <YYYYYY></p> <p>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.</p>
	<p>DEFAULT ELEMENT REFERENCE STATE SYMBOL INDEX /#/: <INDEX></p> <p>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.</p> <p>The index is to define the symbol printed in parameter listings. The symbol can be:</p> <ul style="list-style-type: none"> • 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. <p> 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.</p>

7.3 AMEND_PARAMETER

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 the [ENTER_PARAMETER](#) command for details.

This AMEND_PARAMETER command is for the GES module. There is also a PARROT module command with the same name ([AMEND_PARAMETER](#)).

Syntax	AMEND_PARAMETER
Prompts	<p>PARAMETER: <PARAMETER NAME></p> <p>Specify a correct parameter name. If a parameter name is not acceptable or you only press <Enter>, the error message displays:</p> <p>ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</p> <p>The program prompts for separate input for each part for a parameter name.</p>
	<p>IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK></p> <p>Specify one of these legal identifiers as described for ENTER_PARAMETER.</p> <p>PHASE NAME (/ABCD/): <PHASE NAME></p> <p>Specify the phase name.</p> <p>CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME></p> <p>Specify the constituent name.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME></p> <p>Specify the interacting constituent name: If there is no interacting constituent, press <Enter>.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME></p> <p>If there are more than one interacting constituents, specify them; otherwise press <Enter>.</p> <p>DEGREE /#/ : <DEGREE></p> <p>Specify a numerical number as the degree of the phase parameter.</p>
	<p>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:</p> <pre>L (PHASE2, AL, MG; 1) = 298.15<T<2000.00: +5000 2000.00<T<4500.00: +4500 4500.00<T<6000.00: +4000</pre> <p>Then you are prompted to change the parameter definition, as shown below:</p> <p>DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: <Y OR N></p> <p>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.</p>

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:
```

The previous function is available for editing. The editing is performed within the general subroutine FOOLED, as described in the [AMEND SYMBOL](#) command. This routine prompts as follows:

```
1:+:>
```

The prompt consists of the current position in the string and the character at that position between colons, (::).

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.

7.4 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.

This section outlines the application of each option and includes important information about each command. The next section lists the prompts and subprompts available for each command.

7.4.1 Solution Models in the GIBBS Module

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 in 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 G_m^{ord} 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 $[1-2X(B)]$ 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. Example 52 in the [Thermo-Calc Console Mode Examples](#) (available on the website) specifically demonstrates the use of mixed excess binary models.

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).



See Example 52 in the [Thermo-Calc Console Mode Examples](#) file.

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.



Two examples concerning this Quasichemical Model can be found in the [Thermo-Calc Console Mode Examples](#) files on the website (examples 49 and 50).

QUASICHEM_IRSID

To use the Kapoor-Frohberg-Gaye Quasichemical Cell Model (i.e. the Quasichemical Model developed by IRSID, 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.

7.4.2 Prompts and Options

Syntax	AMEND_PHASE_DESCRIPTION
Prompt	PHASE NAME: <PHASE NAME> Specify the name of the phase. AMEND WHAT /COMPOSITION_SET/: <SUBJECT>

	<p>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.</p> <p>Enter a question mark at the prompt to get a list of all possibly amended subjects for a phase.</p>
	<p>There are no additional prompts for DEBYE_HUCKEL, HKF_ELECTROSTATIC, GLASS_TRANSITION, QUASICHEM_FACT00, QUASICHEM_ISRID, REMOVE_ADDITION, and DEFAULT_STABLE</p>

Option	Description
RENAME_PHASE	<p>NEW PHASE NAME /ABCD/: <PHASE NAME></p> <p>Give a new phase name for the chosen phase, or press <Enter> to keep the default shown.</p>
SITE_RATIOS	<p>SITES IN FIRST SUBLATTICE /XX/ : <YY> SITES IN SECOND SUBLATTICE /XX/ : <YY></p> <p>Specify the site numbers for each of the prompted sublattices for the current phase. Press <Enter> to accept the previous definitions.</p>
NEW_CONSTITUENT	<p>SUBLATTICE /#/: <SUBLATTICE NUMBER></p> <p>Specify the sublattice where the new constituents are located.</p> <p>SPECIES: <SPECIES NAME></p> <p>Give a valid species name.</p>
COMPOSITION_SETS	<p>NEW HIGHEST SET NUMBER /#/: <SET NUMBER N></p> <p>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.</p> <p> You cannot take away the first composition set.</p> <p>MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AB/: <MAJOR CONSTITUENT(S)></p> <p>Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept the default which was automatically set according to the specified composition set of the phase.</p>

Option	Description
	<p>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.</p>
MAJOR_CONSTITUENT	<p>COMPOSITION SET /1/: <COMPOSITION SET NUMBER></p> <p>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.</p> <p>MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AB/: <MAJOR CONSTITUENT(S)></p> <p>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.</p> <p>This prompt is repeated for all available sublattices in the chosen phase for the specified composition set.</p> <p>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.</p>
FRACTION_LIMITS	<p>ELEMENT : <EL1></p> <p>LOW FRACTION LIMIT /0/ : <APPROPRIATE LOW LIMIT></p> <p>HIGH FRACTION LIMIT /1/ : <APPROPRIATE HIGH LIMIT ></p> <p>ELEMENT : <EL2></p> <p>LOW FRACTION LIMIT /0/ : <APPROPRIATE LOW LIMIT></p> <p>HIGH FRACTION LIMIT /1/ : <APPROPRIATE HIGH LIMIT></p> <p>ELEMENT : <ELN></p> <p>LOW FRACTION LIMIT /0/ : <APPROPRIATE LOW LIMIT></p> <p>HIGH FRACTION LIMIT /1/ : <APPROPRIATE HIGH LIMIT ></p>


Option	Description
MAGNETIC_ORDERING	<p>THE ANTIFERROMAGNETIC FACTOR /XX/: <YY></p> <p>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.).</p> <p>SHORT RANGE ORDER FRACTION OF THE ENTHALPY /XX/: <YY></p> <p>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.</p> <p>The default value (xx) is 0.40 for BCC phase, and 0.28 for all other phases (FCC, HCP, etc.).</p>
DISORDERED_PART	<p>DISORDERED PHASE NAME: <PHASE NAME></p> <p>Give the disordered phase name for which there is no ordering sublattice.</p>
EXCESS_MODEL	<p>MODEL NAME /ABCDEFG/: <MODEL NAME></p> <p>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:</p> <ul style="list-style-type: none"> • REDLICH-KISTER_MUGGIANU • REDLICH-KISTER_KOHLER • FLORY-HUGGINS POLYMER MODEL • MIXED-EXCESS-MODELS (R-K default) • HKF • PITZER • CENTRAL_ATOM_MODEL <p>The MIXED-EXCESS-MODELS option has sub-options:</p> <p>FIRST (THE INDEPENDENT) CONSTITUENT: <CONSTITUENT NAME></p> <p>SECOND (THE DEPENDENT) CONSTITUENT: <CONSTITUENT NAME></p> <p>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).</p>

Option	Description
	<p>You are repeatedly prompted with the first sub-option (i.e. <i>First (the independent) constituent</i>) 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).</p> <p>EXCESS MODEL TYPE: /LEGENDRE/: <DESIRED BINARY EXCESS MODEL TYPE></p> <p>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 <i>First (the independent) constituent</i>: 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.</p>
TERNARY_EXTRAPOLAT	<p>EXTRAPOLATION METHOD: /TOOP-KOHLER/: <TERNARY MODEL></p> <p>Choose a ternary extrapolation model for the current solution phase:</p> <ul style="list-style-type: none"> • TOOP-KOHLER for Toop-Kohler Extrapolation Model • KOHLER-ALL for Kohler Extrapolation Model • MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model <p>The TOOP-KOHLER option further prompts:</p> <p>CONSTITUENT IN SUBLATTICE #: <BASIS CONSTITUENT NAME></p> <p>FIRST INTERACTION CONSTITUENT: <INTERACTING CONSTITUENT NAME></p> <p>TOOP CONSTITUENT: <TOOP CONSTITUENT NAME></p> <p>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.</p>

Option	Description
QUASICHEM_IONIC	<p>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.</p> <p>NUMBER OF BONDS/ATOM /2/: <NUMBER OF BONDS PER ATOM></p> <p>Specify the Z value (number of bonds per atom).</p>
STATUS_BITS	<p>Correct the phase status bits. It is important to fully understand this command before using it:</p> <p>NEW STATUS WORD (IN HEXADECIMAL) /04204000/: <NEW STATUS BITS></p> <p>See the command LIST STATUS 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 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.</p>

7.5 AMEND_SYMBOL

Interactively calculate the current values of a function or table (predefined by the switched database or previously entered by the [ENTER SYMBOL](#) command) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.


 This command is also the same when used with the PARROT module. Also, the current values of the temperature and pressure used to calculate the functions or tables are the ones listed in the [LIST STATUS](#) command. 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
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Prompt	<p>NAME: <SYMBOL NAME></p> <p>Specify the name of an entered symbol.</p> <p>For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the <code>Parameter</code> 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:</p> <pre> FUNCTION VALUE 2.52500000E+01 TABLE VALUE 1.56000000E+02 </pre> <p>For variables and functions (or parameters), there are additional prompts and depend on the symbol type.</p> <p>For a variable, its current value is displayed, and you can change it to a new value:</p> <p>VALUE /CURRENT VALUE/: <NEW VALUE></p> <p>For a function (or a parameter entered as a symbol):</p> <p>DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: <Y OR N></p> <p>To change the number of ranges for the function, or change some of the temperature limits in the definition, For <code>Y</code>, you must retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.</p> <p>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:</p> <pre> DIFFERENT FUNCTIONS IN THESE RANGES 298.15<T<2000.00 2000.00<T<4500.00 4500.00<T<6000.00 </pre> <p>and this message displays:</p> <p>DO YOU WANT TO CHANGE RANGE LIMITS /NO/: <Y OR N></p> <p>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 <code>0</code> to exit this command without making any change.</p> <p>RANGE NUMBER (0 TO EXIT) /0/: <RANGE NUMBER></p> <p>FUNCTION:</p> <p>The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:</p> <p>1:+:></p> <p>The prompt consists of the current position in the string and the character at that position between colons (:).</p> <p>These commands can be given:</p>
--------	---

	<ul style="list-style-type: none"> • 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 <p>where CP 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 E at the prompt.</p>
--	--

7.6 CHANGE_STATUS

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 by the LIST_STATUS command.

Syntax	CHANGE_STATUS
Prompt	<p>FOR ELEMENT, SPECIES OR PHASE /SPECIES/: <KEYWORD> Specify the keyword (element, species or phase).</p> <p>SUSPEND /Y/: <Y OR N> The status is changed from ENTERED to SUSPENDED (Y), or vice versa (N).</p> <p>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.</p> <p>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;</p>

7.7 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 v_A, respectively. Initially, these are suspended but can be entered either by this command or the [CHANGE STATUS](#) command.

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	<p>ELEMENT NAME: <ELEMENT NAME></p> <p>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.</p>



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 [REINITIATE](#) command, which removes all data, and should be executed before any other command.

7.8 ENTER_PARAMETER



For the PARROT Module, this command is the same and is described here.

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 rather 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](#)). 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.

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](#).

7.8.1 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 $\omega_{Pr,Tr}$ for aqueous solute species).
- VO: Molar volume at 298.15 K and 1 bar (a numeric value only);
- VA: Integrated thermal expansivity; $\int_{298.15}^T \alpha(T) dT$
- 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](#) or [LIST_PHASE_DATA](#)). 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 $[1\sum y(\text{specified constituents})]$, 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.

Syntax	ENTER_PARAMETER
Prompt	<p>PARAMETER: <PARAMETER NAME></p> <p>As explained above, specify a correct and complete parameter name, which should contain all the necessary parts of the general form:</p> <p><IDENTIFIER> (<PHASE>, <CONSTITUENT ARRAY>; <DIGIT>)</p> <p>If a parameter name is not acceptable or <Enter>, is pressed, the error message displays:</p> <p>*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</p> <p>You are prompted for input for each required part for a parameter name.</p>

Options	Description or additional information
IDENTIFIER	<p>IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK></p> <p>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.</p>

Options	Description or additional information
PHASE NAME	<p>PHASE NAME (/ABCD/) : <PHASE NAME></p> <p>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.</p>
CONSTITUENT	<p>CONSTITUENT (IN SUBLATTICE # /ABC/) : <SPECIES NAME></p> <p>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.</p> <p> It is the species name, not the stoichiometric formula required here.</p> <p>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.</p>
INTERACTING CONSTITUENT	<p>For phases with several sublattices, the program asks for one constituent in each sublattice.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/) : <SPECIES NAME></p> <p>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.</p> <p> To cancel the default value of the interacting constituent type NONE or the name of another constituent.</p> <p>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.</p>
DEGREE	<p>DEGREE /#/: <DEGREE></p> <p>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 (\mathcal{L}), Curie temperature (T_C) and Bohr magneton number (B_{MAGN}), as well as for volume-related parameters (V_0, V_A, V_B, V_C or V_K).</p> <p>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.</p> <p>For a standard G parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.</p>

Options	Description or additional information
PHASE PARAMETER	<p>After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.</p> <p>LOW TEMPERATURE LIMIT /298.15/: <LOWEST TEMPERATURE LIMIT IN K></p> <p>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.</p> <p>FUNCTION: <DEFINITION FOR A FUNCTION></p> <p>A TP-Function consists of terms in T and P.</p> <p>& <CONTINUATION OF THE DEFINITION FOR THE CURRENT FUNCTION></p> <p>Continuation of a TP-Function definition.</p> <p>HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K></p> <p>Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the <i>lowest limit</i> is entered as a negative number) for the current TP-Function.</p> <p>ANY MORE RANGES /N/: <Y OR N></p> <p>Enter Y for more function(s) or N to end this command.</p>

7.9 ENTER_PHASE

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](#) and [AMEND_PHASE_DESCRIPTION](#), which 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](#). In some cases, specify a phase interactively.

7.9.1 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 T_C 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.

7.9.2 About the 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. $G(\text{phase}, A:B:B:B)$, $G(\text{phase}, B:A:B:B)$, $G(\text{phase}, B:B:A:B)$ and $G(\text{phase}, B:B:B:A)$, 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 a bit 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 $G(\text{phase}, A:A:B:B)$ term has 4 nearest neighbour bonds between A and B atoms, whereas the end-member described by the $G(\text{phase}, A:B:A:B)$ 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 $G(\text{phase}, A:A:B:B)$ term) represents B2- ordering and the second (described by the $G(\text{phase}, A:B:A:B)$ term) stands for B32-ordering. There are two permutations of the $G(\text{phase}, A:A:B:B)$ term and four permutations of the $G(\text{phase}, A:B:A:B)$ term, automatically conducted in the Four Substitutional-Sublattice Ordering Model. And there are also two kinds of reciprocal interaction parameters, i.e.

$$L(\text{phase}, A, B : C, D : * : * ; 0 \dots 9) \quad L(\text{phase}, A, B : * : C, D : * ; 0 \dots 9)$$

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

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
		PHASE_B32
		PHASE_D03
		PHASE_L21
HCP PHASE	PHASE_A3	PHASE_D019
		PHASE_B19

7.9.3 Console prompts and options


Syntax	ENTER_PHASE
--------	-------------

Options	Description and additional 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. <input checked="" type="checkbox"/> 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>

Options	Description and additional information
	<p>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.</p> <p>NUMBER OF SITES ON SUBLATTICE # /1/: <SITE NUMBER></p> <p>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 recommended to use integer numbers as sites if possible. For substitutional phases with no sublattices, this question does not show up.</p>
CONSTITUENTS	<p>NAME OF CONSTITUENT: <CONSTITUENT NAME(S)></p> <p>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.</p> <p>WILL YOU ADD CONSTITUENTS LATER /NO/: <Y OR N></p> <p>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>.</p> <p>If illegal constituents are used, you get a message e.g. when parameters are entered.</p> <p>DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: <Y OR N></p> <p>Enter Y for a list of all possible parameters up to the fifth interaction order for the entered phase.</p>

7.10 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.


Examples of species names:

```

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.

Syntax	ENTER_SPECIES
Prompt	<p>SPECIES NAME: <SPECIES NAME></p> <p>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.</p> <p>STOICHIOMETRY /SPECIES NAME/: <CHEMICAL FORMULA></p> <p>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.</p> <p>In upper case mode (see the REINITIATE command), 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.</p> <p> All elements in a species must be entered prior to entering the species.</p>

7.11 ENTER_SYMBOL

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](#)) 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.

A symbol can be entered by this command in the GIBBS module. The symbols entered in the GIBBS module can also be listed and used in the PARROT module (for data optimization) where you can use the GIBBS-entered symbols (variables, functions or parameters) to define parameters that shall be optimized. But symbols entered in the GIBBS module are not the same symbols as defined in the POLY and POST modules.





Also see [ENTER_SYMBOL](#) for the POLY and POST modules.



See example 44 in the [Thermo-Calc Console Mode Examples](#) for an example of using variables and functions.

Syntax	ENTER_SYMBOL
Prompt	<p>VARIABLE, FUNCTION, TABLE OR PARAMETER? /FUNCTION/: <KEYWORD></p> <p>The keyword can be a variable, function, table or parameter.</p> <ul style="list-style-type: none"> 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. <p>NAME: <NAME OF THE SYMBOL></p> <p>Each symbol has a unique name that must start with a letter and can have maximum 8 characters.</p> <p>The following prompts are based on the type of symbol.</p>

Keyword	Description
Variable symbol	<p>VALUE: <NUMERIC VALUE OF A VARIABLE></p> <p>Only a constant numeric value, not an expression, is accepted.</p>
Function symbol	<p>Enter the lower-temperature limit, the expression, an upper-temperature limit and if there is another expression above this upper limit:</p> <p>LOW TEMPERATURE LIMIT /298.15/: <LOWEST TEMPERATURE LIMIT IN K></p> <p>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.</p> <p>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).</p>

Keyword	Description
	<p>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.</p> <p>FUNCTION: <DEFINITION FOR A TP-FUNCTION></p> <p>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.</p> <p> 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).</p> <p>This question is repeated if the current function has more than one expression (TPFunction) in various temperature ranges [or pressure ranges; only if the <i>lowest limit</i> is entered as a negative number)].</p> <p>& <CONTINUATION OF THE DEFINITION FOR THE CURRENT TP-FUNCTION></p> <p>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.</p> <p>HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K></p> <p>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.</p> <p>This question is repeated if the function has more than one expression (TPFunction) in various temperature ranges.</p> <p> 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.</p>

Keyword	Description
	<p>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.</p> <p>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.</p> <p>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.</p> <p>ANY MORE RANGES /N/: <Y OR N></p> <p>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.</p> <p>Important note: Make sure that the function and its first derivatives are continuous across break points.</p>
Table symbol	<p>Specify the low and high temperature limits, temperature step and tabled value at each specified temperature:</p> <p>LOW TEMPERATURE LIMIT /298.15/: <LOW TEMPERATURE LIMIT IN K></p> <p>The lowest temperature where the table has a value.</p> <p>HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K></p> <p>The highest temperature where the table has a value.</p> <p>STEP IN TEMPERATURE /100/: <TEMPERATURE STEP></p> <p>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.</p> <p>TABLE VALUE AT XX /YY/: <TABLE VALUE></p> <p>The value of the table at the specified temperature (xx) must be given. The default value (yy) is the last value.</p>

Keyword	Description
Parameter symbol	<p>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 command or the Function symbol prompts above.</p> <p>PARAMETER: <PARAMETER NAME></p> <p>Specify a correct and complete parameter name, which should contain all the necessary parts of the general form:</p> <p><IDENTIFIER> (<PHASE>, <CONSTITUENT ARRAY>; <DIGIT>)</p> <p>If a parameter name is not acceptable or <Enter> is pressed, this error message displays:</p> <p>*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</p> <p>The program prompts for separate input for each required part for a parameter name.</p> <p>IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK></p> <p>Specify one of these types of legal identifiers.</p> <p>PHASE NAME (/ABCD/): <PHASE NAME></p> <p>Specify the phase name.</p> <p>CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME></p> <p>Specify the constituent name on the specified sublattice site of the given phase.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME></p> <p>Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME></p> <p>If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.</p> <p>DEGREE /#/ : <DEGREE></p> <p>Specify an integer number (a value from 0 through 9) as the degree for the phase parameter.</p> <p>LOW TEMPERATURE LIMIT /298.15/: <LOWEST TEMPERATURE LIMIT IN K></p> <p>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.</p> <p>FUNCTION: <DEFINITION FOR A FUNCTION></p>

Keyword	Description
	<p>Specify the desired TP-Function for the current temperature range (or current pressure range; only if the <i>lowest limit</i> is entered as a negative number).</p> <p>& <CONTINUATION OF THE DEFINITION FOR THE CURRENT TP-FUNCTION></p> <p>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).</p> <p>HIGH TEMPERATURE LIMIT /6000/: <HIGH TEMPERATURE LIMIT IN K></p> <p>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.</p> <p>ANY MORE RANGES /N/: <Y OR N></p>

7.12 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.

Syntax	LIST_CONSTITUENT
--------	------------------

7.13 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
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME></p> <p>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>).</p> <p>OPTIONS?: <OPTION(S)></p>

	<p>Choose one or several of these options for output:</p> <ul style="list-style-type: none"> • 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.
--	---

7.14 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
Prompt	<p>PARAMETER: <PARAMETER NAME></p> <p>Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)</p> <p>Examples of parameter names, the identifiers are described in PARAMETER NAME.</p> <p>If a parameter name is not acceptable or <Enter> is pressed, an error message displays:</p> <p>*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</p> <p>The program prompts for separate input for each required part for a parameter name.</p> <p>IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK></p> <p>Specify one of these types of legal identifiers.</p> <p>PHASE NAME (/ABCD/): <PHASE NAME></p> <p>Specify the phase name.</p> <p>CONSTITUENT (IN SUBLATTICE # /ABC/): <SPECIES NAME></p> <p>Specify the constituent name on the specified sublattice site of the given phase.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME></p>

	<p>Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): <SPECIES NAME></p> <p>If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.</p> <p>DEGREE /#/ : <DEGREE></p> <p>Specify a numerical number as the degree for the phase parameter.</p>
--	--

7.15 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.

Syntax	LIST_PHASE_DATA
Prompt	<p>PHASE NAME: <PHASE NAME></p> <p>Specify a phase name (if abbreviated, it should be unique).</p>

 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.

7.16 LIST_STATUS

List the entered elements, phases and species with the status word. The command is included for system managers.

Syntax	LIST_STATUS
--------	-------------

Important

Each element, species, phase and symbol has a set of status bits. The values of these bits are listed with this command. These are not normally of interest but the meaning is explained here.

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.

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)

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)

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


Set Symbol Status Word (*Bit meaning*) if:

1. Constant
2. Variable
3. Function
4. Table
5. Value must not be amended
6. Undefined

7.17 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
Prompt	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>).

7.18 READ_GES_WORKSPACE


The data area saved onto a *.GES5 file by a [SAVE_GES_WORKSPACE](#) command is read back into the GIBBS 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).


Syntax	READ_GES_WORKSPACE
--------	--------------------

 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.

7.19 REINITIATE

All data in the stored GIBBS workspace are erased, and all variables are initiated to their default values.

Syntax	REINITIATE
Prompt	<p>UPPER CASE ONLY /Y/: <Y OR N></p> <p>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).</p> <p> In upper case mode all input in lower case is automatically converted to upper case.</p> <p>LOWER TEMPERATURE LIMIT /298.15/: <LOWEST T IN K></p> <p>This value is used as the lower temperature limit when data are entered interactively.</p> <p>UPPER TEMPERATURE LIMIT /6000/: <HIGHEST T IN K></p> <p>This value is used as the upper temperature limit when data are entered interactively.</p> <p>DEFAULT ELEMENT REFERENCE STATE SYMBOL INDEX /1/: <1 OR 2 OR 3></p> <p>Specify a proper index for the default listing parameters (symbol), or press <Enter> to accept the preset index 1.</p> <p>The <i>index</i> is for defining the symbol printed in listings of parameters. The symbol can be:</p> <ul style="list-style-type: none"> • G: the data are referred to Gibbs energy at a variable temperature (also called <i>Lattice Stability</i>). • 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.

7.20 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](#) 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.

7.21 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
Prompt	<p>VALUE OF GAS CONSTANT IN YOUR ENERGY UNITS /8.31451/: <NEW VALUE></p> <p>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.</p> <p>VALUE OF ONE BAR IN YOUR PRESURE UNITS /100000/: <NEW VALUE></p> <p>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.</p>

8. PARROT Commands

- [AMEND_PARAMETER](#)
- [AMEND_SYMBOL](#)
- [COMPILE_EXPERIMENTS](#)
- [CONTINUE_OPTIMIZATION](#)
- [CREATE_NEW_STORE_FILE](#)
- [EDIT_EXPERIMENTS](#)
- [ENTER_PARAMETER](#)
- [LIST_ALL_VARIABLES](#)
- [LIST_CONDITIONS](#)
- [LIST_PARAMETER](#)
- [LIST_PHASE_DATA \(from GIBBS\)](#)
- [LIST_RESULT](#)
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- [LIST_SYMBOL_IN_GES](#)
- [OPTIMIZE_VARIABLES](#)
- [READ_PARROT_WORKSPACES](#)
- [RECOVER_VARIABLES](#)
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- [SET_ALTERNATE_MODE](#)
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- [SET_FIX_VARIABLE](#)
- [SET_OPTIMIZING_CONDITION](#)
- [SET_OPTIMIZING_VARIABLE](#)
- [SET_OUTPUT_LEVELS](#)
- [SET_SCALED_VARIABLE](#)
- [SET_STORE_FILE](#)

8.1 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](#)).

Syntax	AMEND_PARAMETER
Prompt	<p>PARAMETER: <PARAMETER NAME></p> <p>Specify a correct parameter name. If a parameter name is not acceptable or <Enter> is pressed, the error message displays:</p> <p>*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</p> <p>The program prompts for separate input for each part for a parameter name.</p> <p>IDENTIFIER (/X/): <G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK></p>

Specify one of these types of legal identifiers (see [ENTER_PARAMETER](#) for details).

```
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  
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 the [AMEND_SYMBOL](#) command. This routine prompts as follows:

```
1:+:>
```

The prompt consists of the current position in the string and the character at that position between colons, (: :).

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.

```
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.

8.2 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 the CREATE-NEW-STORE-FILE command, set by the SET_STORE_FILE command, or opened with the READ_PARROT_WORKSPACE command, all done before the COMPILE_EXPERIMENTS command.

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.



For more information about DATAPLOT search the online help or refer to the *DATAPLOT User Guide* on the website.

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.	
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <*.POP FILE NAME></p> <p>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.</p> <p>INITIATE STORE FILE /Y/: <Y OR N></p> <p>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.</p> <p>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.</p>

8.3 CONTINUE_OPTIMIZATION

This command continues the optimization using the same Hessian matrix.



In some cases it is illegal 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
PROMPT	ARE YOU SURE? /N/: <N OR Y>

	<p>Prior to this question, a message displays to confirm if it is OK to continue:</p> <pre> It is safe to CONTINUE only after TOO MANY ITERATIONS and no change in variables and experiments ... Now anything can happen ... </pre> <p>You can accept the default (N) in order to cancel this special attempt.</p> <p>NUMBER OF ITERATIONS /N/: <INTEGRAL NUMBER OF ITERATION></p> <p>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.</p>
--	---

8.4 CREATE_NEW_STORE_FILE

Create a binary file to be used as a *work* file (or 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.



This file is hardware dependent and cannot be read by any text editor.

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
	<p><*.PAR FILE NAME></p> <p>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.</p>

8.5 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.



See [Running the EDIT_EXPERIMENTS Command](#) for information.

Syntax	EDIT_EXPERIMENTS
--------	------------------

8.6 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, see [SET_OUTPUT_LEVELS](#).

Syntax	LIST_ALL_VARIABLES
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME></p> <p>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.</p>

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

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

```

8.7 LIST_CONDITIONS

List the values of the output and optimizing conditions, either on screen or in a basic text file which can be opened and edited by a text editor.

Syntax	LIST_CONDITIONS
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME></p> <p>A list of the current values of optimization conditions, as well the current status of listing, in the PARROT workspace is written on screen (by pressing <Enter>) or on the list file under a specific file name.</p>

8.8 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	<p>PHASE NAME: <PHASE NAME></p> <p>Specify a phase name.</p>

8.9 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 [SET_OUTPUT_LEVELS](#) command.

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**.

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;
- 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).

Syntax	LIST_RESULT
Prompt	FULL, CONDENSED, DETAILED OR GRAPHIC FORMAT: /C/: <C OR D OR F OR G>
	<p>Choose a format.</p> <ul style="list-style-type: none"> • 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. <p>OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME></p> <p>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.</p>

Example Output



The following is the listed result in the example TCEX36 (See example 36 in the [Thermo-Calc Console Mode Examples](#)), after the first optimization based on the prescribed definitions in the TCEX36a.TCM and TCEX36b.TCM, but having set all variables available for optimization.

```
*** 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;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
5.00E+02 -6.561 -1.3122E-02 -1957.

```

8.10 LIST_STORE_FILE


Displays the name of the store file and its full path.

Syntax	LIST_STORE_FILE
--------	-----------------

8.11 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.

8.12 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	<p>NUMBER OF ITERATION /N/: <INTEGRAL NUMBER OF ITERATION></p> <p>Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT program tries this number of different sets of values of the optimizing variables unless it has converged earlier, or has given up earlier.</p> <p> 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 the LIST_RESULT command to check how good (bad) the current fit is.</p>

8.13 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.

The previous PARROT/GIBBS/POLY3 workspaces are always associated with the latest action to either open a work file by the [SET_STORE_FILE](#) command, or to create a work file by the [CREATE_NEW_STORE_FILE](#) command (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file), or to update the work file by the [SAVE_PARROT_WORKSPACES](#) command.

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.

You cannot use this command if there is no work file opened or created already.

Syntax	READ_PARROT_WORKSPACE
--------	-----------------------

8.14 RECOVER_VARIABLES

The values of all variables are set back to the start values.

Syntax	RECOVER_VARIABLES
--------	-------------------

8.15 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.



This command should never be used, unless you really want to destroy the current PARROT workspace. However, this PARROT command does not reinitiate the GIBBS/POLY3 workspaces.

Syntax	REINITIATE
--------	------------

8.16 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.

Syntax	RESCALE_VARIABLES
--------	-------------------

8.17 SAVE_PARROT_WORKSPACES

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 the [SET_STORE_FILE](#) command or been created by the [CREATE_NEW_STORE_FILE](#) command (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.

Syntax	SAVE_PARROT_WORKSPACE
--------	-----------------------

8.18 SET_ALTERNATE_MODE

Turn the alternate mode on or off. The alternate mode is described in [PARROT Commands](#). 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.

8.19 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.

Notes

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

8.20 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 the SET_OPTIMIZING_VARIABLE command.


Syntax	SET_FIX_VARIABLE
Prompt	<p>VARIABLE NUMBER: <VARIABLE NUMBER(S)></p> <p>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).</p> <p>START VALUE /XXXX.XXXXX/: <A VALUE TO BE FIXED></p> <p>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 shown as default.</p> <p>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.</p>

8.21 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.

Syntax	SET_OPTIMIZING_CONDITION
Prompt	<p>RELATIVE STANDARD DEVIATION FOR EXPERIMENTS? /N/: <Y OR N></p> <p>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.</p> <p>MIN SAVE ON FILE? /Y/: <Y OR N></p> <p>Specify whether the program should minimize the transfer of data to and from the current work file during the optimization:</p> <p>If Y, it speeds up the optimization. After optimization use the SAVE_PARROT_WORKSPACE command to update the progress onto the current work file.</p> <p>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.</p>

	<p>ERROR FOR VARIABLE BOUNDS: /1/: <RETURN ></p> <p>This feature has not been implemented yet. Press <Enter>.</p> <p>RELATIVE STEP FOR CALCULATION OF DERIVATIVES: /1E-04/: <XXX></p> <p>In the calculation of the correlation matrix for equilibria with inaccuracy in the independent state variables, some numerical derivatives might have to be calculated.</p> <p>Specify the relative step (xxx) for the calculation of these derivatives.</p> <p>MAXFUN (VA05AD): /100/: <N></p> <p>The maximum number of iterations in the optimization. The same value set by the OPTIMIZE command.</p> <p>DMAX (VA05AD): /100/: <N></p> <p>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.</p> <p>H (VA05AD): /1E-04/: <XXX></p> <p>The step used in the scaled variables for calculating numerical derivatives during the optimization.</p> <p>ACC/(INITIAL SUM OF SQUARES) (VA05AD): /.001/: <XXX></p> <p>The break condition for the optimization. The accepted value is the difference between the true minimum and the calculated one.</p>
--	---

 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.


8.22 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 the [SET_FIX_VARIABLE](#) command 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 the LIST_ALL_VARIABLE command.

Syntax	SET_OPTIMIZING_VARIABLE
Prompt	<p>VARIABLE NUMBER: <VARIABLE NUMBER(S)></p> <p>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.</p>

	<p>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.</p> <p>START VALUE /XXXX.XXXXX/: <A GUESS VALUE></p> <p>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.</p>
--	--

 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.

8.23 SET_OUTPUT_LEVELS


Choose the type of information the PARROT module gives during the optimization procedure and when listing results.

Syntax	SET_OUTPUT_LEVELS
Prompt	<p>LIST INCREMENT /1/: <INCREMENT IN ITERATION NUMBER></p> <p>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.</p> <p>LIST SUM OF SQUARES: /Y/: <Y OR N></p> <p>Choose whether the sum of squares is listed on screen during the optimization procedure.</p> <p>LIST SCALED VARIABLES: /Y/: <Y OR N></p> <p>Choose whether the scaled variable values are listed on the terminal during the optimization procedure.</p> <p>LIST WEIGHTENED RESIDUALS: /N/: <N OR Y></p> <p>Choose whether the weighted residuals are listed on the terminal during the optimization procedure.</p> <p>LIST ALL PARAMETERS: /N/: <N OR Y></p> <p>Choose whether all parameters in the models are listed at the LIST_RESULT command.</p> <p>LIST CORRELATION MATRIX: /N/: <N OR Y></p> <p>Choose whether the correlation matrix of the variables are listed at the LIST_RESULT and LIST_ALL_VARIABLES commands.</p>

8.24 SET_SCALED_VARIABLE

This command is similar to the [SET_OPTIMIZING_VARIABLE](#) command 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 the [SET_FIX_VARIABLE](#) command 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 the [LIST_ALL_VARIABLES](#) command.

Syntax	SET_SCALED_VARIABLE
Prompt	<p>VARIABLE NUMBER: <VARIABLE NUMBER(S)></p> <p>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.</p> <p>START VALUE /XXXX.XXXXX/: <A GUESS VALUE></p> <p>Specify a start guess of the optimum value. The current numerical value for the selected variable is shown as default.</p> <p> This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria.</p> <p>MIN VALUE /XXXX.XXXXX/: <A GUESS VALUE></p> <p>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.</p> <p>MAX VALUE /XXXX.XXXXX/: <A GUESS VALUE></p> <p>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.</p>

8.25 SET_STORE_FILE

Specify a store file (work file) to be used for compilation and optimization. The *.PAR work file must be created (by the CREATE-NEWSTORE-FILE command) 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	<p>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.</p>

9. POLY_3 Commands

- [ADD_INITIAL_EQUILIBRIUM](#)
- [ADVANCED_OPTIONS](#)
- [AMEND_STORED_EQUILIBRIA](#)
- [CHANGE_STATUS](#)
- [COMPUTE_EQUILIBRIUM](#)
- [COMPUTE_TRANSITION](#)
- [CREATE_NEW_EQUILIBRIUM](#)
- [DEFINE_COMPONENTS](#)
- [DEFINE_DIAGRAM](#)
- [DEFINE_MATERIAL](#)
- [DELETE_INITIAL_EQUILIBRIUM](#)
- [DELETE_SYMBOL](#)
- [ENTER_SYMBOL](#)
- [EVALUATE_FUNCTIONS](#)
- [LIST_AXIS_VARIABLE](#)
- [LIST_CONDITIONS](#)
- [LIST_EQUILIBRIUM](#)
- [LIST_INITIAL_EQUILIBRIA](#)
- [LIST_STATUS](#)
- [LIST_SYMBOLS](#)
- [LOAD_INITIAL_EQUILIBRIUM](#)
- [MAP](#)
- [POST](#)
- [READ_WORKSPACES](#)
- [RECOVER_START_VALUES](#)
- [REINITIATE_MODULE](#)
- [SAVE_WORKSPACES](#)
- [SELECT_EQUILIBRIUM](#)
- [SET_ALL_START_VALUES](#)
- [SET_AXIS_VARIABLE](#)
- [SET_CONDITION](#)
- [SET_INPUT_AMOUNTS](#)
- [SET_NUMERICAL_LIMITS](#)
- [SET_REFERENCE_STATE](#)
- [SET_START_CONSTITUTION](#)
- [SET_START_VALUE](#)
- [SHOW_VALUE](#)
- [STEP_WITH_OPTIONS](#)
- [TABULATE](#)

9.1 ADD_INITIAL_EQUILIBRIUM

Add initial equilibrium points from which a phase diagram is calculated (through the MAP command).

Normally, this command is not needed to calculate a property diagram (through the STEP NORMAL command-sequence). In many cases, the ADD_INITIAL_EQUILIBRIUM 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_EQUILIBRIUM 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 the `LIST_INITIAL_EQUILBRIUM` command. A certain initial equilibrium point (including its conditions and equilibrium results) can be loaded into the current equilibrium, if needed, by the `LOAD_INITIAL_EQUILBRIUM` command. Any specific or all of the initial equilibrium points can be deleted from current POLY workspace, if desired, by the `DELETE_INITIAL_EQUILBRIUM` command.

Syntax	ADD_INITIAL_EQUILBRIUM
Prompt	<p>DIRECTION /DEFAULT/: <DIRECTION CODE></p> <p>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.</p> <p>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.</p>

9.2 ADVANCED_OPTIONS

These options can be set:

```
POLY_3:adv
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
```

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 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 the advanced option 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 by the [SET_AXIS_VARIABLE](#) command.

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 starting bulk composition for the system.

Always set the status of the chosen interstitial components as SPECIAL using the POLY command: `CHANGE_STATUS 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 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_VALUE 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 T_0 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.

Syntax	ADVANCED_OPTIONS
Prompt	WHICH OPTION? /STEP_AND_MAP/: <OPTION>

Options	Description or additional information
NONE	<p>Take away any set advanced option in all subsequent single-point equilibrium and MAP/STEP calculations.</p> <p>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:</p> <pre>Convergence problems, increasing smallest site-fraction from 1.00E-30 to hardware precision</pre>

Options	Description or additional information
	<p>2.00E-14. You can restore using SET-NUMERICAL-LIMITS</p> <p>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 to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.</p>
STEP_AND_MAP (the default)	<p>Settings for MAP and STEP:</p> <p>GLOBAL TEST INTERVAL /0/: <INTEGER NUMBER></p> <p>Settings for MAP:</p> <p>AUTOMATICALLY ADD INITIAL EQUILIBRIA /Y/: <Y OR N></p> <p>NUMBER OF MESH ALONG AN AXIS /3/: <INTEGER NUMBER></p> <p>USE INSIDE MESHING POINTS /N/: <Y OR N></p> <p>GLOBAL TEST INTERVAL /0/: <INTEGER NUMBER></p> <p>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 <i>n</i>-th 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 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.</p> <p>AUTOMATICALLY ADD INITIAL EQUILIBRIA /Y/: <Y OR N></p>

Options	Description or additional information
	<p>When the ADD_INITIAL_EQUILIBRIUM command 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.</p> <p>NUMBER OF MESH ALONG AN AXIS /3/: <INTEGER NUMBER></p> <p>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.</p> <p>USE INSIDE MESHING POINTS /N/: <Y OR N></p> <p>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.</p>
EQUILIBRIUM_CALCUL	<p>The following prompts affect the ways how the POLY optimization does the Ordinary POLY Minimization to reach the minimum of an equilibrium state.</p> <p>Settings for the minimization of an equilibria:</p> <p>FORCE POSITIVE DEFINITE PHASE HESSIAN /Y/: <Y OR N></p> <p>CONTROL STEPSIZE DURING MINIMIZATION /Y/: <Y OR N></p> <p>FORCE POSITIVE DEFINITE PHASE HESSIAN /Y/: <Y OR N></p> <p>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].</p>


Options	Description or additional information
	<p>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.</p> <p>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.</p> <p>By answering N the Ordinary POLY Minimization routine is applied.</p> <p>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:</p> $G_m(X) = G_m(T, P; y_1, y_2, \dots, y_n)$ <p>Compute a Hessian matrix as which describes the curvature of the Gibbs energy curve of this phase at the defined composition X:</p> $\partial^2 G_m / \partial y_i \partial y_j$ <p>Diagonalise this matrix and call the Eigenvalues as e_1, e_2, \dots, e_n. The QF(phase) quantity for this phase is the lowest of these eigenvalues divided by the same values for a corresponding ideal (stoichiometric) phase:</p> $QF(ph) = \min(\{e_1, e_2, \dots, e_n\}) / \min(\{se_1, se_2, \dots, se_n\})$ <p>Here, se_1, se_2, \dots, se_n are the eigenvalues for the ideal phase. Therefore, for an ideal (stoichiometric) phase, the QF(phase) should always be 1.0.</p> <p>CONTROL STEPSIZE DURING MINIMIZATION /Y/: <Y OR N></p>

Options	Description or additional information
	<p>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.</p>
GLOBAL_MINIMIZATION	<p>The following prompts affect how the Global Minimization is done. Settings for global minimization:</p> <p>USE GLOBAL MINIMIZATION AS MUCH AS POSSIBLE /Y/: <Y OR N></p> <p>USE GLOBAL MINIMIZATION FOR TEST ONLY? /N/: <Y OR N></p> <p>MAXIMUM NUMBER OF GRIDPOINTS PER PHASE /2000/: <INTEGER NUMBER></p> <p>USE GLOBAL MINIMIZATION AS MUCH AS POSSIBLE /Y/: <Y OR N></p> <p>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.</p> <p>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 reached. This costs more computer time but the calculations are more accurate.</p> <p>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.</p> <p>USE GLOBAL MINIMIZATION FOR TEST ONLY? /N/: <Y OR N></p> <p>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.</p>

Options	Description or additional information
	<p>If <code>N</code> 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.</p> <p>MAXIMUM NUMBER OF GRIDPOINTS PER PHASE /2000/: <INTEGER NUMBER></p> <p>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.</p>
IGNORE_COMPOSI_SET_ORDER	IGNORE COMPOSITION SET ORDER /N/
NEW_COMPOSITION_SET	<p>The following prompts are to specify the additional composition set(s) to handle possible miscibility gap(s) of a certain solution phase:</p> <p>PHASE WITH MISCIBILITY GAP: <NAME OF A PHASE></p> <p>Specify the name of the phase with miscibility gap.</p> <p>NEW HIGHEST COMPOSITION SET NUMBER /2/: <#></p> <p>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.</p> <p>A message displays to show that you need to specify the composition for the composition set # (2,3,...).</p> <p>MAJOR CONSTITUENT(S) FOR SUBLATTICE 1: /XX/: <YY></p> <p>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 should have different major constituents for each composition set.</p>

Options	Description or additional information
	<p>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.</p>
MAJOR_CONSTITUENT	<p>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:</p> <p>PHASE NAME: <NAME OF A PHASE></p> <p>Specify the name of the solution phase with a new set of major constituents.</p> <p>COMPOSITION SET NUMBER /1/: <#></p> <p>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.</p> <p>MAJOR CONSTITUENT(S) FOR SUBLATTICE 1: /XX/: <YY></p> <p>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.</p> <p>This question is repeated for each sublattice in the phase.</p>
PHASE_ADDITION	<p>The following prompts are to specify the additional energy term (always being a constant) of a given phase.</p> <p>PHASE NAME: <NAME OF A PHASE></p> <p>Specify the name of the (stoichiometric or solution) phase with the addition.</p> <p>ADDITION TO G PER MOLE FORMULA UNIT: <XXXXX></p> <p>The value (xxxxxx) 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.</p> <p><input checked="" type="checkbox"/> It is not composition-, temperature- or pressure-dependent.</p>
LIST_PHASE_ADDITION	No additional prompt.

Options	Description or additional information
PRESENT_PHASE	<p>Specify the name of the present phase a the name of the phase that should be present at all calculated equilibria:</p> <p>PRESENT PHASE:</p> <p>PHASE NAME: <NAME OF A PHASE></p>
T-ZERO TEMPERATURE	<p>NAME OF FIRST PHASE: <PHASE A></p> <p>NAME OF SECOND PHASE: <PHASE B></p> <p>The names of phases A and B must be given, for which the T_0 temperature (where the Gibbs energies are equal) is to be calculated.</p> <p>If the T_0 temperature between the two specified phases is successfully calculated, a message displays, e.g.</p> <p>THE T_0 TEMPERATURE IS 840.82 K. NOTE: LIST-EQUILIBRIUM IS NOT RELEVANT</p> <p>The first message shows the calculated T_0 temperature between the two specified phases.</p> <p>The second indicates that after this option calculation the LIST_EQUILIBRIUM command is irrelevant and does not list the equilibrium for the system at the T_0-temperature.</p>
PARAEQUILIBRIUM	<p>NAME OF FIRST PHASE: <PHASE A></p> <p>NAME OF SECOND PHASE: <PHASE B></p> <p>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.</p>

Options	Description or additional information
	<p> 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.</p> <p>FAST DIFFUSING COMPONENT: /C/: <INTERSTITIAL COMPONENT(S)></p> <p>FAST DIFFUSING COMPONENT: /NONE/: <INTERSTITIAL COMPONENT(S)></p> <p>The name(s) of the fast-diffusing component(s) (C as the default single 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.</p> <p>Note the following:</p> <p>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;</p> <p>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;</p>

Options	Description or additional information
	<p>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);</p> <p>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;</p> <p>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.</p> <p>If the paraequilibrium state between the two specified phases is successfully calculated, the messages displays e.g.</p> <pre> 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 </pre> <p>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.</p>

Options	Description or additional information
	<p>However, if the single-point calculation of the paraequilibrium state between the two specified phases has failed, these messages display:</p> <pre>*** ERROR 4 IN NS01AD *** NUMERICAL ERROR</pre> <p>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.</p>
STABILITY_CHECK	<p>STABILITY CHECK ON? /Y/: <Y OR N></p> <p>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.</p> <p>CHECK ALSO FOR UNSTABLE PHASES? /Y/: <Y OR N></p> <p>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 gap 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.</p>
TOGGLE_ALTERNATE_MODE	<p>SET ALTERNATE TOGGLE TO DEFAULT, ALWAYS, OR NEVER?</p> <p>SET GLOBAL TOGGLE TO DEFAULT, ALWAYS, OR NEVER?</p>

Options	Description or additional information
	<p>DEFAULT means that the experiment points are calculated according to the Alternate Technique depending on the SET_ALTERNATE command.</p> <p>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.</p> <p>NEVER means the experiment points are calculated as normal equilibria even if you SET_ALTERNATE in the PARROT module.</p>
SHOW_FOR_T=	<p>TEMPERATURE (K) /298.15/: <TEMPERATURE_IN_K></p> <p>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 various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system (being in a <i>frozen</i> state) is shown on screen.</p> <p>STATE VARIABLE OR SYMBOL /VM/: <STATE VARIABLE OR SYMBOL NAME(S)></p> <p>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).</p>
OUTPUT FILE FOR SHOW	<p>A window opens with a default name for the file <code>tc_show.dat</code>. Choose a location to save the file and click Open.</p>

9.3 AMEND_STORED_EQUILIBRIA

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
Prompt	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>

	<p>Y restore everything.</p> <p>RANGE: <RANGE(S) OF REGION></p> <p>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.</p> <p>In order to know the ranges the LIST option must first be used.</p> <p>S(USPEND) K(EEP) /K/: <S OR K></p> <p>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.</p> <p>OUTPUT FILE: /SCREEN/: <FILE NAME></p> <p>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.</p>
--	--

9.4 CHANGE_STATUS


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 *ufractions* 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.

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 statuses:

- **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.

Syntax	CHANGE_STATUS
Prompt	<p>FOR PHASES, SPECIES OR COMPONENTS? /PHASES/: <KEYWORD></p> <p>KEYWORD = phase or species or components</p> <p>PHASE NAME(S) : <NAME(S) OF THE PHASE(S)></p> <p>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 assigned to the phases can also be given on the same line if preceded with an equal sign =.</p> <p> 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.</p> <p>NAME(S) : <NAME(S) OF THE SPECIE(S) OR COMPONENT(S)></p> <p>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 =.</p>

 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 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 $NPF(\text{phase})$ 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, $NP(\text{phase})$, $BP(\text{phase})$ and $VP(\text{phase})$, 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 $NPF(\text{phase})$.

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
```

```
= 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 +
```

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.

	<p>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.</p> <p>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).</p> <p>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</p> $N/[p + q^*y_C^2 + q^*y_N^2 + q^*y_{O^2}^2 + q^*y_{FeO^{2-3/2}}].$
--	--

9.5 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 MINIMIZATION_OPTION command-sequence. Also search the online help and see the *Thermo-Calc User Guide* for more information.

Syntax	COMPUTE_EQUILIBRIUM
--------	---------------------

Notes

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 (by the LIST_STATUS CPS command-sequence) and equilibrium conditions (by the LIST_CONDITION command) and list out the calculation results (by the LIST_EQUILIBRIUM command), 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.

See also the POLY command [SET NUMERICAL LIMITS](#) 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 has not been found, an error message is given on screen. In such a case, you may try to repeat this command a few times, or to 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.

9.6 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 [CHANGE STATUS](#) command 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` calculation to assure the calculated transitional equilibrium is a really stable one, and can also use the `LIST_EQUILIBRIUM` command to see the details of transitional equilibrium state.

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.

Syntax	<code>COMPUTE_TRANSITION</code>
Prompt	<p>PHASE TO FORM: <PHASE NAME></p> <p>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 <code>FIXED</code> as 0 amount, and the program shows the information such as:</p> <pre> You must remove one of the these conditions P=100000, T=800, N=1, X(Fe)=.5 DEGREE OF FREEDOM 0 </pre>

It is also possible to find out any new phase to be formed in a certain direction of the released condition if the key word **ANY** is given as the phase name when it is prompted for Phase to form. In such a case, the above is displayed.

```
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 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
```

9.7 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
Prompt	<p>EQUILIBRIUM NUMBER /2/: <A NEW EQUILIBRIUM NUMBER></p> <p>Each equilibrium in the POLY3 workspace is identified by a unique integer number. Such an equilibrium number can be recalled by the SELECT_EQUILIBRIUM command later on.</p> <p>INITIATION CODE /2/:</p> <p>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.</p> <p> The entered components and phases can later be changed with the CHANGE_STATUS command.</p>


9.8 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 command implies a REINITIATE_MODULE command and it should be given as the first command in the POLY module.

Syntax	DEFINE_COMPONENTS
Prompt	<p>GIVE ALL NEW COMPONENTS /EXISTING COMPONENTS/: <NEW COMPONENTS></p> <p>The new components must be specified all on one line. These replace the existing component definitions.</p> <p> The number of components cannot be changed with this command. Use CHANGE_STATUS instead.</p>

	<p>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.</p> <p> The new components do not have to be present as species.</p>
--	--

9.9 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 the normal SET_AXIS_VARIABLE command in the sequent POST monitor.

Syntax	DEFINE_DIAGRAM
Prompt	<p>These prompts are given:</p> <p>SAME ELEMENTS AS BEFORE /Y/? <Y OR N></p> <p>MOLE PERCENT OF <ELEMENT> /##/: <VALUE></p> <p>OR</p> <p>MASS PERCENT OF <ELEMENT> /##/: <VALUE></p> <p>DATABASE /ABCDE/: <DATABASE NAME></p> <p>MAJOR ELEMENT OR ALLOY: <ELEMENT NAME></p> <p>COMPOSITION IN MASS (WEIGHT) PERCENT? /Y/: <Y OR N></p>

```

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 the
DEFINE_MATERIAL command. 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>

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
/#/: <##>

```

	<p>Select one of the independent conditions or dependent quantities as the Y-axis variable, by giving its corresponding index given on the condition lists.</p> <p> It must be different from the X-axis variable already selected.</p> <p>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.</p> <p>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.</p> <p>NAME OF PHASE: /ABC/: <PHASE NAME></p> <p>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.</p> <p>MULTIPLE START POINTS? /Y/: <Y OR N></p> <p>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.</p> <p>SAVE FILE /RESULT/: <FILE NAME></p> <p>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).</p>
--	--

9.10 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 by the LIST_EQUILIBRIUM command 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
Prompt	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.

 The `DEFINE_MATERIAL` 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.

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` 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>

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 (°C).

 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 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>
```

	<p>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).</p> <p>By pressing <Enter>, the DEFINE_MATERIAL command starts calculating the equilibrium, and then is terminated.</p> <p>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.</p> <p>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).</p> <p>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 major element composition limit.</p>
--	--

9.11 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; see also the [ADD_INITIAL_EQUILIBRIUM](#) command.

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 the LIST_INITIAL_EQUILIBRIA command to figure out the numbers for all the existing initial equilibrium points that have already been added (<i>manually</i> through the ADD_INITIAL_EQUILIBRIUM command, or <i>automatically</i> by some other POLY commands) and stored in the current POLY3 workspace. By default, ALL the initial equilibrium points are deleted.
--	---

9.12 DELETE_SYMBOL

Delete symbols (i.e. constants, variables, functions or tables. These symbols are entered by the command ENTER_SYMBOL.

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.

9.13 ENTER_SYMBOL

Symbols are a useful feature of POLY and POST to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can even 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 a STEP_WITH_OPTIONS command) or mapping calculation (enforced by a MAP command). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using the EVALUATE_FUNCTIONS command 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](#) for the GIBBS module.



See example 44 in the [Thermo-Calc Console Mode Examples](#) for an example of using variables and functions.

Syntax	ENTER_SYMBOL
Prompt	CONSTANT, VARIABLE, FUNCTION OR TABLE? /FUNCTION/: <KEYWORD>

The **keyword** can be 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 these may depend on each other.

Variables are similar to functions because these can also be expressions of state variables. However, contrary to functions, these are only evaluated when entered or if they are explicitly named in an EVALUATE command. It is possible to enter a variable with a new expression anytime. 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 stand for a definition of temperature in Celsius. Otherwise, these questions are asked.



For different types of symbols (constant, function, variable or table) the questions are different.

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
```

The temperature in Celsius

```
T-273.15
```

```
<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 calculation 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 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.

9.14 EVALUATE_FUNCTIONS

The value of one or more or all entered functions or variables are evaluated and listed.

 Variables are evaluated only if these are explicitly named.

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.

9.15 LIST_AXIS_VARIABLE

All the axis variables for a stepping or mapping calculation that have already been set by the [SET_AXIS_VARIABLE](#) command are listed.

Syntax	LIST_AXIS_VARIABLE
--------	--------------------


9.16 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 the SET_CONDITION or CHANGE_STATUS command. 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 output	P=100000, T=800, N(NI)=1E-1, N=1 FIXED PHASES FCC_A1=1 LIQUID=0 DEGREE OF FREEDOM 0

9.17 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	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME></p> <p>The name of the text file where the list of the calculation results shall be written.</p> <p>OPTIONS /VWCS/: <OPTION(S)></p> <p>Select the output units and formats by optionally specifying a combination of these letters.</p> <ul style="list-style-type: none"> <i>Fraction order:</i> V means VALUE ORDER; A means ALPHABETICAL ORDER. <i>Fraction type:</i> W means MASS FRACTION; X means MOLE FRACTION. <i>Composition:</i> C means only COMPOSITION; N means CONSTITUTION and COMPOSITION. <i>Phase:</i> S means including only STABLE PHASES; P means including ALL NON-SUSPENDED PHASES. <p>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).</p> <p>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 <code>L_E, , ,</code> or <code>LIST_EQUILIBRIUM , , ,</code></p> <p> <code>LIST_EQUILIBRIUM</code> displays <code>ORD</code> (ordered) or <code>DISORD</code> (disordered) (when available). See CHANGE LEGEND for details.</p>

9.18 LIST_INITIAL_EQUILIBRIA

List all the equilibria added with the [ADD_INITIAL_EQUILIBRIUM](#) command. All the initial equilibria are used for the MAP (and STEP) calculations.

Syntax	LIST_INITIAL_EQUILIBRIA
--------	-------------------------

9.19 LIST_STATUS


List the status of components, species or phases.

Results

Depending upon the key word specified in the [CHANGE_STATUS](#) options, a table with the current status of phases or species or components, or their combinations, is shown:

- For components, the statuses and reference states are 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.

For species, only the status is listed.

Syntax	LIST_STATUS
Prompt	Specify what to list: OPTION /CPS/: <KEYWORD(S)> KEYWORD = C OR P OR S, OR ANY COMBINATION <ul style="list-style-type: none"> C means list component status P means list phase status S means list species status CS for both components and species Default is CPS.

9.20 LIST_SYMBOLS

For both the POLY and POST modules, list the definitions for all constants, functions, variables and tables. The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %.

In order to find the value of a function or variable, use the SHOW or EVALUATE commands. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
--------	--------------

9.21 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 the LIST_INITIAL_EQUILIBRIA command.

9.22 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](#). 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 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](#) 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 the `ADD_INITIAL_EQUILIBRIUM` command) inside various phase-region boundaries under certain direction(s).

9.23 POST

Switch to the post-processor (the POST module), which has its own command repertoire. See [POST Commands](#) for all details.

Syntax	POST
--------	------

9.24 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 a `SAVE_WORKSPACES` command. Such an *.POLY3 file is not printable.

Syntax	READ_WORKSPACES
Options	<p>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.</p> <p>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.</p>

	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 <code>READ, ,</code> or <code>READ_WORKSPACE , ,</code>
--	---

9.25 RECOVER_START_VALUES

Recover the start values in equilibrium calculations.

Syntax	RECOVER_START_VALUES
--------	----------------------


9.26 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. 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.

Syntax	REINITIATE_MODULE
--------	-------------------

9.27 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.

Syntax	SAVE_WORKSPACES
Options	<p>A <code>file name</code> must be specified. The default extension of the POLY workspace file is *.POLY3 (Windows) or *.poly3 (Linux), while you can have any other extension.</p> <p>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.</p> <p> 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 <code>SAVE, , y</code> or <code>SAVE_WORKSPACE , , y</code>. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.</p>

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.


9.28 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	<p>NUMBER /NEXT/: <CHOICE ON EQUILIBRIUM></p> <p>Answer FIRST, LAST, NEXT, PREVIOUS or PRESENT.</p> <p>Most commands affect only the PRESENT equilibrium. However, the REINITIATE MODULE and DEFINE_COMPONENT commands remove all the stored equilibria.</p>

9.29 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
Prompt	<p>T /XXXX/: <TEMPERATURE IN K></p> <p>If the temperature is not a condition, supply a guess of its final value (in K).</p> <p>P /100000/: <PRESSURE IN PA></p> <p>If the pressure is not a condition supply a guess of its final value (in pa).</p> <p>AUTOMATIC START VALUES FOR PHASE CONSTITUTIONS? /N/: <Y, N OR F></p> <p>Answer N (the default), Y or F (for force).</p> <p>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.</p> <p>If Y this command immediately terminates, and the program automatically sets the start values for phase constitutions in all possible phases.</p> <p>For N supply an initial amount of each entered phase and the major constituents or site fraction of each constituent.</p> <p>SHOULD <PHASE> BE STABLE /N/: <Y/1 OR N/2></p> <p>A guess on if this phase should be stable or not is requested. All entered phases are prompted for this question and next two.</p> <p> 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).</p> <p>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.</p> <p>MAJOR CONSTITUENT(S) : <NAME OF MAJOR CONSTITUENT(S) IN THE PHASE></p>

	<p>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.</p> <p>Y (<PHASE>, <CONSTITUENT>) / .XXXXXXXXXX/ : <.YYYYY></p> <p>The current value (.XXXXXXXXXX) is default. You can accept the default by pressing <Enter> or give a new value (.YYYYY).</p> <p>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.</p>
--	---

9.30 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.

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.

Syntax	<code>SET_AXIS_VARIABLE</code>
Prompt	<p><code>AXIS NUMBER /#/: <AN AXIS NUMBER></code></p> <p>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.</p> <p><code>CONDITION /NONE/: <ONE CONDITION></code></p> <p>Here the condition that should be varied along the axis must be given. The condition is specified as in the <code>SET_CONDITION</code> command, for example <code>W(C)</code> for mass fraction of carbon. By accepting <code>NONE</code>, the axis is removed.</p> <p><code>MIN VALUE /0/: <MIN VALUE></code></p> <p>Specify the minimum value of the axis condition.</p> <p><code>MAX VALUE /1/: <MAX VALUE></code></p> <p>Specify the maximum value of the axis condition.</p> <p><code>INCREMENT /.025/: <STEP LENGTH></code></p> <p>Specify the maximum step length. By default, this is 1/40 of the total axis length.</p>

9.31 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 (through the [CHANGE STATUS](#) command), it is equivalent to one condition (implying that particular phase is stable in the defined system).

Syntax	<code>SET_CONDITION</code>
	<p>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.</p> <p>Example:</p> <pre>SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,CR)=.22, ACR(N)=.2</pre> <p>or</p>

	<pre>SET_COND T=1273, P=1E5</pre> <pre>SET_COND W(C)=.0015, X(LIQ,CR)=.22 ACR(N)=.2</pre> <p>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.</p>
Prompt	<p>STATE VARIABLE EXPRESSION: <STATE VARIABLE NAME OR LINEAR EXPRESSION> OR A LINEAR EXPRESSION OF STATE VARIABLES.</p> <p>Some of the state variables that can be used in conditions are:</p> <ul style="list-style-type: none"> • 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) <p>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. For example,</p> <pre>T=1273.15 P=1E5</pre> <pre>X(C)=.002</pre> <pre>W(CR)=0.5</pre> <pre>ACR(CR)=0.85</pre> <pre>X(FCC,C)=.001</pre> <pre>H=-250000</pre> <pre>HM(BCC)=-225000</pre> <p>A condition can also be a value of a linear expression involving more than one state variable. For example,</p> <pre>X(LIQ,S)-X(PYRR,S)=0</pre>

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 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.

9.32 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
```



You can give negative amounts in the SET-INPUT-AMOUNTS command.

Syntax	SET_INPUT_AMOUNTS
Prompt	<p>QUANTITY: <N(<SPECIE>) OR B(<SPECIE>)></p> <p>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.</p> <p>AMOUNT: <VALUE OF THE QUANTITY></p> <p>Specify the numerical value of the quantity.</p>

9.33 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 the COMPUTE_EQUILIBRIUM, STEP_WITH_OPTION, MAP or ADVANCED_OPTIONS commands), 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	<p>MAXIMUM NUMBER OF ITERATIONS /200/: <XXX></p> <p>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.</p> <p>REQUIRED ACCURACY /1E-6/: <YYY></p> <p>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.</p> <p>SMALLEST FRACTION /1E-12/: <ZZZ></p> <p>This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.</p>

	<p>The default value for the smallest site-fractions is $1\text{E}-12$ 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 $1\text{E}-30$ (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. $1\text{E}-45$, that is naturally enforced to all the phases in the system).</p> <p>APPROXIMATE DRIVING FORCE CALCULATION FOR METASTABLE PHASES /Y/: <Y OR N></p> <p>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.</p>
--	--


9.34 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
Prompt	<p>COMPONENT: <NAME OF THE COMPONENT></p> <p>The name of the component must be given.</p> <p>REFERENCE PHASE: <NAME OF A PHASE USED AS THE NEW REFERENCE STATE></p> <p>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.</p> <p>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.</p> <p>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.</p> <p> The actual calculation of the reference state is only performed when SET_REFERENCE_STATE is executed.</p> <p>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.</p> <p>TEMPERATURE /*/: <TEMPERATURE FOR THE REFERENCE STATE></p> <p>Select the temperature (in K) for the reference state. The wildcard value * means the current temperature is used for the calculation.</p> <p>PRESSURE /1E5/: <PRESSURE FOR THE REFERENCE STATE></p> <p>Select the pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for the calculation.</p>
Examples	<pre> S-R-S Fe SER S-R-S Cr FCC * 100000 S-R-S H2O AQUEOUS * 100000 S-R-S ZE REF_ELECTRODE * 100000 </pre>


9.35 SET_START_CONSTITUTION

This command is similar to the SET-ALL-START-VALUES command, but is used for an individual phase that may have a wrong constitution.

Syntax	SET_START_CONSTITUTION
Prompt	<p>PHASE NAME: <NAME OF A PHASE, AND POSSIBLE MAJOR CONSTITUENT(S)></p> <p>Specify the name of a phase for which the constitution shall be set.</p> <p>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.</p> <p>Y (<PHASE>#<COMPOSITION_SET>,<CONSTITUENT>#<SUBLATTICE>) /XXX/: <SF></p> <p>The site fraction (SF) of the constituent shall be given. The default value xxx is the last calculated one.</p>

9.36 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
Prompt	<p>STATE VARIABLE: <NAME OF A STATE VARIABLE></p> <p>The state variable must be given.</p> <p>VALUE:</p> <p>Specify the value to be assigned the state variable as start value.</p>

9.37 SHOW_VALUE


Show the current value of any state variable, function or variable.

Syntax	SHOW_VALUE
Prompt	<p>STATE VARIABLE OR SYMBOL: <NAME(S) OF STATE VARIABLE(S) OR SYMBOL(S)></p> <p>A single or several state variables or symbols (entered functions or variables) can be specified.</p>

	<p> 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 <code>SHOW W(*,*)</code> lists the mass fraction of all phases, whereas <code>SHOW W(\$,*)</code> lists the mass fraction of all stable phases.</p> <p> If you <code>SHOW</code> a function, all functions are evaluated using the current values of the state variables. But if you <code>SHOW</code> a variable, it retains its value from the time it was <code>ENTERED</code> or last <code>EVALUATED</code>. Therefore to save a value from one calculation to another, <code>ENTER</code> it to a variable. This is frequently done in the <code>PARROT</code> module to transfer values between equilibria.</p>
--	---

9.38 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) that is set by the `SET_AXIS_VARIABLE` command.

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 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	<p>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).</p> <p> 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.</p> <p>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.</p>

Options	Choose from these options
	<p>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:</p> <p>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.</p> <p>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.</p> <p>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 MAP calculation) for the same system.</p>


Options	Choose from these options
INITIAL_EQUILIBRIA	<p>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.</p>
SEPARATE_PHASES	<p>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 G_m 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.</p>


Options	Choose from these options
ONE_PHASE_AT_TIME	<p>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.</p> <p>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 heterogeneous systems with both ordered phases and their disordered pairs.</p>
EVALUATE	<p>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.</p> <p>Specify the prompt:</p> <p>VARIABLE NAME (S) : <VARIABLE NAME></p> <p>The names of the variables that shall be evaluated after each step must be typed here.</p> <p>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) if a phase has two or more composition sets.</p>


Options	Choose from these options
	<p>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.</p> <p>One good case of using this advanced option is described in the INFORMATION command 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.</p> <p> See example 30A in the Thermo-Calc Console Mode Examples. Or go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations.</p>
MIXED_SCHEIL	<p>Extended Scheil-Gulliver type solidification with back diffusion.</p> <p>This option leads to a stepping calculation (always with T as the stepping axis variable) for simulating Extended Scheil-Gulliver solidification processes (i.e. <i>partial-equilibrium transformations</i>) 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.</p> <p>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:</p> <p>For solution phases with possibility of miscibility gap existence, you have appropriately added the necessary composition set(s);</p> <p>You have already set the temperature condition as the stepping</p>


Options	Choose from these options
	<p>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.</p> <p>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].</p> <p>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.</p> <p>With this stepping calculation option, these prompts need to be specified:</p> <pre>FAST DIFFUSING COMPONENTS: <FAST DIFFUSION INTERSTITIAL(S)></pre> <p>Specify one or more interstitial component(s) as the back-diffusion component(s).</p> <p>If there is only one fast-diffusing interstitial component (e.g. C or N), type its name at the prompt;</p> <p>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);</p> <p>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.</p>

Options	Choose from these options
	<p><input checked="" type="checkbox"/> 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.</p> <p>ALLOW BCC -> FCC ? /Y/: <Y OR N></p> <p>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).</p> <p>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 (N_L, mole fraction), overall formed solid phases (N_S, mole fraction) and latent heat formation (N_H, J/mol) along the cooling process are shown after the information on starting temperature point of the alloy solidification process, e.g.</p> <pre> 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 1733.1500 0.3294 0.6707 -8032.6240 1733.0250 0.3237 0.6763 -8095.1490 </pre>


Options	Choose from these options
	<p>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 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 (N_S in mole-fraction or B_S in mass-fraction), the amount of remaining liquid phase (N_L in mole-fraction or B_L in mass fraction), the heat of latent along the solidification process (N_H in J/mol or B_H in J/gram), among many other properties in the solidified alloy phases or in the whole alloy system.</p> <p>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.</p>
T-ZERO	<p>T0 lines between two specific phases calculated This option allows a stepping calculation of the so-called T0 (T-zero) line in a <i>diffusionless transformation</i> [where two specific partially-equilibrated phases have the same Gibbs energy, along a composition variable which has already set as the stepping variable by the SET_AXIS_VARIABLE command.</p> <p> The temperature condition cannot be set as the stepping variable if you want to make a STEP T-ZERO calculation.</p> <p>To ensure a successful calculation of T_0 line between two specific phases after an initial equilibrium calculation in the current system, it is recommended to make a single T_0 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.</p> <p>Specify these prompts:</p> <p>NAME OF FIRST PHASE: <PHASE A></p>

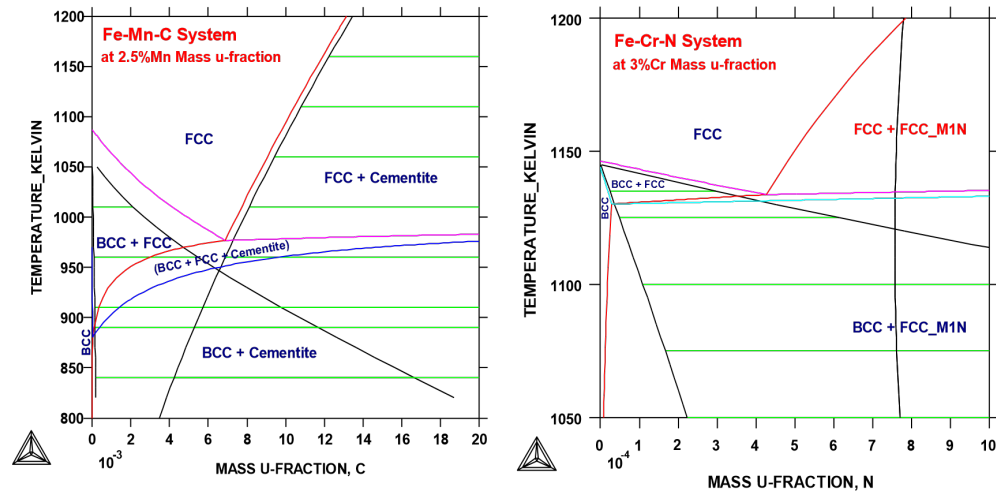
Options	Choose from these options
	<p>NAME OF SECOND PHASE: <PHASE B></p> <p>The names of the two target phases, for which the Gibbs energies equal to each other at each point on the T_0 line, must be typed at the above two prompts subsequently.</p> <p>During the STEP T-ZERO calculation procedure, the calculated T_0 values are shown after the corresponding scanned conditions (of the stepping composition variable), e.g.</p> <pre> 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 </pre> <p>After a successful STEP T-ZERO calculation, you can go to the POST module to plot the T_0 line against the stepping composition variable or another varying axis, or to impose the calculated T_0 line onto a normal phase diagram [normally plotted as a T-X isopleth].</p> <p> See Examples 23 and 41 in the Thermo-Calc Console Mode Examples.</p>
PARAEQUILIBRIUM	<p>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.</p>

Options	Choose from these options
	<p>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 by the SET AXIS VARIABLE command.</p> <p>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.</p> <p> The composition condition for the interstitial components cannot be set as the stepping variable if you want to make a STEP PARAEQUILIBRIUM calculation.</p> <p>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.</p> <p>Always check if the chosen <code>phaseA</code> and <code>phaseB</code> 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).</p>


Options	Choose from these options
	<p>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 starting bulk composition for the system.</p> <p>Always set the status of the chosen interstitial components as SPECIAL using the command:</p> <pre>CHANGE_STATUS COMPONENT <interstitial component> = SPECIAL</pre> <p>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.</p> <p>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.</p> <p>With this stepping calculation option, these prompts need to be specified:</p> <pre>NAME OF FIRST PHASE: <PHASE A> NAME OF SECOND PHASE: <PHASE B></pre> <p>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).</p> <p> It is important to understand that this is the calculation of a paraequilibrium state between the two specified phases.</p> <p>Particularly, there are four issues which need to be considered:</p> <ol style="list-style-type: none"> 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


Options	Choose from these options
	<p>and interstitial components of the current alloy system; or</p> <p>4. It is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.</p> <p>FAST DIFFUSING COMPONENT: /C/: <INTERSTITIAL COMPONENT(S)></p> <p>FAST DIFFUSING COMPONENT: /NONE/: <INTERSTITIAL COMPONENT(S)></p> <p>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.</p> <p>Note the following:</p> <p>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.</p> <p>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;</p> <p>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);</p> <p>To finish the input of fast-diffusing elements, accept NONE at a repeated prompt;</p> <p>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.</p> <p>During the STEP PARAEQUILIBRIUM calculation procedure, the calculated paraequilibrium states include the:</p> <ul style="list-style-type: none"> corresponding stepping conditions (e.g. temperature in K, or the stepping composition

Options	Choose from these options
	<p>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);</p> <ul style="list-style-type: none"> • 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))]; • 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). <p>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].</p> <p> See examples 23 and 42 in Thermo-Calc Console Mode Examples.</p> <p>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.</p>



The figure above (the left-hand side plot is from Example 42e) 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](#) 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.

9.39 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
Prompt	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>

10. POST Commands

The POST module (post-processor) is available from the POLY module. See [POLY 3](#) Commands for other information about the POLY module. Read [Using the POST Module](#) before beginning.

- [ADD LABEL TEXT](#)
- [APPEND EXPERIMENTAL DATA](#)
- [CHANGE LEGEND](#)
- [DUMP DIAGRAM](#)
- [ENTER SYMBOL](#)
- [FIND LINE](#)
- [LIST DATA TABLE](#)
- [LIST PLOT SETTINGS](#)
- [LIST SYMBOLS](#)
- [MAKE EXPERIMENTAL DATAFILE](#)
- [MODIFY LABEL TEXT](#)
- [PLOT DIAGRAM](#)
- [PRINT DIAGRAM](#)
- [QUICK EXPERIMENTAL PLOT](#)
- [REINITIATE PLOT SETTINGS](#)
- [RESTORE PHASE IN PLOT](#)
- [SELECT PLOT](#)
- [SET AXIS LENGTH](#)
- [SET AXIS PLOT STATUS](#)
- [SET AXIS TEXT STATUS](#)
- [SET AXIS TYPE](#)
- [SET COLOR](#)
- [SET CORNER TEXT](#)
- [SET DIAGRAM AXIS](#)
- [SET DIAGRAM TYPE](#)
- [SET FONT](#)
- [SET INTERACTIVE MODE](#)
- [SET LABEL CURVE OPTION](#)
- [SET PLOT FORMAT](#)
- [SET PLOT OPTIONS](#)
- [SET PLOT SIZE](#)
- [SET PREFIX SCALING](#)
- [SET RASTER STATUS](#)
- [SET REFERENCE STATE](#)
- [SET SCALING STATUS](#)
- [SET TIC TYPE](#)
- [SET TIELINE STATUS](#)
- [SET TITLE](#)
- [SET TRUE MANUAL SCALING](#)
- [SUSPEND PHASE IN PLOT](#)
- [TABULATE](#)

10.1 Using the POST Module

Use the Post module after a STEP or MAP calculation to generate various *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).

In the Thermo-Calc (and DICTRA) software, 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](#).


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

10.2 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.

 In some cases such an optional calculation for automatic phase region labelling may fail. It is not possible to automatically add labels for certain sets of axes, like entropy, enthalpy, pH, Eh, etc.

The label texts and coordinates, either added by this command or modified by the [MODIFY_LABEL_TEXT](#) command (or manually edited in the **Console Results** window), are stored in the workspace, and these may later be saved onto an *.EXP file (through the MAKE_EXPERIMENTAL_DATAFILE command).

Syntax	ADD_LABEL_TEXT
Prompt	<p>GIVE X COORDINATE IN AXIS UNITS: <VALUE OF THE X COORDINATE></p> <p>Specify the value of the X coordinate where the label is to start.</p> <p>GIVE Y COORDINATE IN AXIS UNITS: <VALUE OF THE X COORDINATE></p> <p> The labels disappear if any axis is changed afterwards.</p> <p>Specify the value of the Y coordinate where the label is to start.</p> <p>AUTOMATIC PHASE LABELS? /Y/: <Y OR N></p> <ul style="list-style-type: none"> 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

	<p>heterogeneous interaction systems; in such cases, a message displays:</p> <p>TEXT: <TEXT FOR THE LABEL></p> <ul style="list-style-type: none"> • 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 Al_2O_3 as subscripts: <pre>\LATEX MOLE-FRACTION AL_2O_3</pre> <p>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:</p> <pre>\ROTATION 45</pre> <p>To rotate the text and use LaTeX, the rotation command must be used first. For example:</p> <pre>\ROTATION 45 \LATEX MOLE-FRACTION AL_2O_3</pre> <p>Rotates the text 45° and includes subscripts in the title Mole-fraction Al₂O₃.</p> <p>TEXT SIZE: /.35/: <SIZE FOR THE LABEL></p> <p>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.</p>
--	--

 These changes to plot labels can also be manually edited in the **Console Results** window. See the *Thermo-Calc Console Mode User Guide* for details.

 For a list of basic LaTeX commands, see <http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html>

10.3 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` (see below), 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.



For more information about DATAPLOT search the online help or refer to the *DATAPLOT User Guide* on the website.

Syntax	APPEND_EXPERIMENTAL_DATA
Prompt	<p>USE EXPERIMENTAL DATA (Y OR N) /N/: <Y OR N></p> <p>Specify whether the data from an experimental data file should be included in the next plot. If the answer is <code>c</code>, no experimental data are plotted.</p> <p>An Open window displays to specify the name of the file with the experimental data.</p> <p>PROLOGUE NUMBER: /0/: <PROLOGUE NUMBER></p> <p>Select which prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on.</p> <p> By answering -1, a list of all prologues on the file is given; and by 0, no experimental data are appended.</p> <p>DATASET NUMBER(S) /-1/: <DATASET NUMBER(S)></p> <p>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.</p>

10.4 CHANGE_LEGEND

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name. See *About Legend Styles* in the *Thermo-Calc User Guide* for detail and examples of these labels.




[LIST_EQUILIBRIUM](#) 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](#) option is set to `F`.


Syntax	CHANGE_LEGEND
Prompt	<p>SET SUFFIX FOR PHASE NAMES IN LEGEND? (ALL, NONE, CONSTITUTION, ORDERING) /NONE/:</p> <p>When you select <code>None</code> the legend includes the standard information about the phases.</p>

	<p>When you select <code>All</code> the Constitution description and the Ordering description (when there is ordering) are also included.</p> <p>When you select <code>Constitution</code>, this is added to the standard description.</p> <p>When you select <code>Ordering</code> and when there is ordering, this is added to the standard description.</p> <p> See <i>About Legend Styles</i> in the <i>Thermo-Calc User Guide</i> for examples of these labels.</p>
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10.5 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 the case for the `PRINT_DIAGRAM` command, 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	<code>DUMP_DIAGRAM</code>
Prompt	<p><code>OUTPUT FORMAT /: <FORMAT OR RETURN></code></p> <p>Specify an appropriate graphic format for dumping the graph or pressing <Enter> to accept the default format.</p> <p>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 (<code>Y</code>) the old file or not (<code>N</code>).</p> <p> 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, so that you can save the graph in file(s) using the <code>PLOT_DIAGRAM</code> command.</p>

10.6 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	<code>FIND_LINE</code>
Prompt	<code>X COORDINATE /.484623611/: <VALUE OF THE X COORDINATE></code>

	<p>Specify the value of the X coordinate where you want to find the details of property curve (or phase region).</p> <p>Y COORDINATE /.5153737962/: <VALUE OF THE Y COORDINATE></p> <p>Specify the value of the Y coordinate where you want to find the details of property curve (or phase region).</p> <p>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).</p>
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10.7 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/manipulated or used for further graphical handling by opening the file (using the MS-Excel program) outside of the Thermo-Calc software system.



It works only for a property diagram after a stepping calculation (but not for any phase diagram after a mapping calculation).

Syntax	LIST_DATA_TABLE
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME OR RETURN ></p> <p>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).</p>

10.8 LIST_PLOT_SETTINGS

List the present values of most parameters specifying the type of diagram to be plotted.

Syntax	LIST_PLOT_SETTINGS
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10.9 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.




For more information about DATAPLOT search the online help or refer to the *DATAPLOT User Guide* on the website.

Syntax	MAKE_EXPERIMENTAL_DATAFILE
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <NAME OF A FILE OR RETURN></p> <p>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).</p>

10.10 MODIFY_LABEL_TEXT

Move a label created with the ADD_LABEL_TEXT command 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 the MAKE_EXPERIMENTAL_DATAFILE command).

Syntax	MODIFY_LABEL_TEXT
Prompt	<p>WHICH LABEL TO MODIFY? /#/ : <NUMBER OF THE LABEL></p> <p>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.</p> <p>NEW X COORDINATE: /XXX/: <NEW X POSITION></p> <p>Specify the new X position. The previous X coordinate is displayed. Press <Enter> to accept.</p> <p>NEW Y COORDINATE: /YYY/: <NEW Y POSITION></p> <p>Specify the new Y position. The previous Y coordinate is displayed. Press <Enter> to accept.</p> <p>NEW TEXT /ABCDEFGH.../: <NEW LABELING TEXT></p> <p>Specify the new labeling text. The previous text is displayed. Press <Enter> to accept.</p> <p> The new label text must not be longer than the previous text.</p>

10.11 PLOT_DIAGRAM

The graphic information is plotted on a specific graphic device using the plot format set by the SET_PLOT_FORMAT command.



The diagram axes must be set first.

The functionality of this command is split up into two: one remained in the PLOT_DIAGRAM command for normal screen display and file saving; and the other implemented in the PRINT_DIAGRAM command (under MS-Windows environment) for direct hard-copy printing.

With this command, a calculated/plotted diagram is displayed if the default graphic device has already been defined, or it can be saved onto a file.

Syntax	PLOT_DIAGRAM
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <NAME OF A FILE OR RETURN FOR SCREEN></p> <p>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.</p> <p>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.</p>

10.12 PRINT_DIAGRAM

To print with high quality to a file. After a Thermo-Calc graph is created (and is displayed with the PLOT_DIAGRAM command)



It has the same function as the Print Plot option on the Console Results windows. Use it to print the plotted diagram to a connected printer (also possible to a fax machine, as a word-editing document or graphical-formatted file, depending upon how you have set your local printer settings).

Syntax	PRINT_DIAGRAM
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10.13 QUICK_EXPERIMENTAL_PLOT

This is similar to the APPEND_EXPERIMENTAL_DATA command 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.



For more information about DATAPLOT search the online help or refer to the *DATAPLOT User Guide* on the website.

Syntax	QUICK_EXPERIMENTAL_PLOT
Prompt	PROLOGUE NUMBER: /0/: <PROLOGUE NUMBER>

	<p>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.</p> <p><code>DATASET NUMBER(S) /-1/: <DATASET NUMBER(S)></code></p> <p>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.</p>
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10.14 REINITIATE_PLOT_SETTINGS

All parameters describing the diagram are given default values. Therefore, all plotting setting made in the POST module is lost, and everything returns to the initial settings when the POST module is entered.

Syntax	REINITIATE_PLOT_SETTINGS
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10.15 RESTORE_PHASE_IN_PLOT

Restores a phase previously suspended from the plot with the SUSPEND_PHASE_IN_PLOT command. It works only after at least one phase is suspended.

Syntax	RESTORE_PHASE_IN_PLOT
Prompt	<p><code>PHASE NAME: <NAME OF A PHASE></code></p> <p>Give the name of the phase to be restored.</p>

10.16 SELECT_PLOT

Select a plot within the current Results tab in the Console Results window.

Syntax	SELECT_PLOT
Prompt	<p><code>PLOT <N/NEW></code></p> <p>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.</p> <p>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.</p>

10.17 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
Prompt	<p>AXIS (X, Y OR Z): <NAME OF AN AXIS></p> <p>Specify which axis to set the length.</p> <p>AXIS LENGTH /11.5/: <NEW RELATIVE AXIS LENGTH></p> <p>Specify the new real axis length in inches. The relative length 1 corresponds to 10 tic-marks on the axis.</p>

10.18 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, the SET_TIC_TYPE command should be used 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	<p>AXIS PLOT (Y OR N) /Y/: (Y OR N)</p> <p>Specify to plot axis texts (Y) or no (N).</p>

10.19 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
Prompt	<p>AXIS (X, Y OR Z): <NAME OF AN AXIS></p> <p>Specify which axis text status to change.</p> <p>AUTOMATIC AXIS TEXT (Y OR N) /N/: <Y OR N></p> <p>Specify if automatic axis text is to be used (Y) or (N). If you answer N, enter axis text:</p> <p>AXIS TEXT: <ENTER AXIS TEXT></p> <p>You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size. See ADD_LABEL_TEXT for information.</p>


10.20 SET_AXIS_TYPE

Change the axis type among linear, logarithmic and inverse axis.

Syntax	SET_AXIS_TYPE
Prompt	<p>AXIS (X, Y OR Z): <NAME OF AN AXIS></p> <p>Specify which axis to change the axis type.</p> <p>AXIS TYPE /LINEAR/: <NEW AXIS TYPE></p> <p>Specify which new axis type to set. Select LINEar (default), LOGarithmic or INverse. Only the three first characters are relevant.</p>

10.21 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	<p>TEXT AND AXIS KEYWORD /DEFAULT OPTION/ <RETURN OR NEW OPTION></p> <p>INVARIANT EQUILIBRIA KEYWORD /DEFAULT OPTION/: <RETURN OR NEW OPTION></p> <p>TIE-LINES COLOR KEYWORD /DEFAULT OPTION/: <RETURN OR NEW OPTION></p> <p>KEYWORD OF ALL OTHER LINES /DEFAULT OPTION/: <RETURN OR NEW OPTION></p> <p>This is usually for the solubility lines.</p>

Notes

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 command); the POST module *automatically* switches on the appropriate **Keyword**.

The legal options for **Color** are: **BACKGROUND**

- **FOREGROUND** (default)
- **RED** (default for invariant equilibria)
- **GREEN** (default for tie lines)
- **BLUE**
- **YELLOW**
- **MAGENTA**
- **CYAN**
- **PURPLE**

- GOLD4
- TURQUOISE4
- PINK
- GRAY
- ORANGERED3
- MAROON
- PLUM
- SEAGREEN
- OLIVEDRAB
- SIENNA
- ORANGE1
- CORAL1
- USERDEF

The legal options for `LineType` are:

- INVISIBLE
- NORMAL (default)
- VERY_THICK (default for invariant equilibria)
- THIN (default for tie lines)
- THICK
- VERY_THIN
- DASHED
- DOTTED

10.22 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_OPTION`, 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	<code>SET_CORNER_TEXT</code>
Prompt	<p><code>CORNER /LOWER_LEFT/: <RETURN OR NEW OPTION></code></p> <p>Choose an option:</p> <ul style="list-style-type: none"> • <code>LOWER_LEFT</code> • <code>UPPER_LEFT</code> • <code>UPPER_RIGHT</code> • <code>LOWER_RIGHT</code> • <code>TOP_OF_TRIANGLE</code> <p><code>TEXT: <TEXTS AS A SUBTITLE OR A NOTE></code></p> <p>Write the texts that are to be written on the specified diagram corner.</p>

10.23 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.

Syntax	SET_DIAGRAM_AXIS
Prompt	<p>AXIS (X, Y OR Z): <AXIS NAME></p> <p>Specify which axis (X or Y or Z) to set with a variable.</p> <p>VARIABLE TYPE: <VARIABLE NAME></p> <p>Specify a variable for the chosen axis here.</p> <p>The valid variables are:</p> <ul style="list-style-type: none"> • TEMPERATURE-CELSIUS as temperature in °C • 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 or Any entered table. <p>If you specify an entered table as the variable, then:</p> <p>FOR COMPONENT: <COMPONENT NAME></p>

	<p>When an activity, mole or weight fraction or percent of a component shall be plotted, the component name must be supplied here.</p> <p>COLUMN NUMBER: <COLUMN NUMBER(S)></p> <p>Specify the column number(s) in the chosen table that are to be plotted onto the earlier specified axis. For example:</p> <ul style="list-style-type: none"> • 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
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Notes

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 command. It simplifies the use of Thermo-Calc and DICTRA, but this option has not been made visually available in Thermo-Calc, because users may believe that they cannot set any other axis than used in the mapping calculation.

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.

10.24 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	<code>SET_DIAGRAM_TYPE</code>
Prompt	<code>TRIANGULAR DIAGRAM (Y OR N) /N/: <Y OR N></code>

	<p>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.</p> <p>CREATE TETRAHEDRON VRML FILE (Y OR N) /N/: <Y OR N></p> <p>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.</p> <p>PLOT 3:RD AXIS (Y OR N) /N/: <Y OR N></p> <p>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.</p> <p>CLIP ALONG 3:RD AXIS (Y OR N) /N/: <Y OR N></p> <p>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).</p>
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10.25 SET_FONT

Select the font to use for labels and numbers when plotting the diagram under the currently selected graphic device (by the SET_PLOT_FORMAT command). For some devices there may be other fonts available and these are selected by the SET_PLOT_FORMAT command.

Syntax	SET_FONT
Prompt	<p>SELECT FONTNUMBER /1/: <#></p> <p>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.</p> <p>FONT SIZE /.34/: <##></p> <p>The size of the chosen font is specified. A value around 0.34 is recommended.</p>

10.26 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.


Syntax	SET_INTERACTIVE_MODE
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10.27 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	<p>CURVE LABEL OPTION (A, B, C, D, E, F OR N) /A/: <OPTION></p> <p>The options:</p> <ul style="list-style-type: none"> • 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 <p>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.</p> <p> 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.</p> <p>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 (by the command SET_DIAGRAM_AXIS Y NP(*)) on the Y-axis versus T-C on the X-axis, then the list may have lines like:</p> <pre>1: T-273.15, NP(LIQUID) 2: T-273.15, NP(FCC_A1)</pre> <p>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.</p>

10.28 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 the SET_PLOT_ENVIRONMENT command in the system monitor or by your TC.INI file.

Syntax	SET_PLOT_FORMAT
Prompt	<p>GRAPHIC DEVICE NUMBER /#/: <NUMBER OF THE DEVICE></p> <p>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 ?.</p> <p>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.</p>

10.29 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
Prompt	<p>PLOT HEADER /Y/: <Y OR N></p> <p>Toggle the plotting of the Thermo-Calc header text above a diagram.</p> <p>PLOT LOGO /Y/: <Y OR N></p> <p>Toggle the plotting of the Thermo-Calc logotype at the lower-left corner of a diagram.</p> <p>PLOT FOOTER /Y/: <Y OR N></p>

	<p>Toggle the plotting of the footer identifier text at the right margin of a diagram.</p> <pre>WHITE-CONTOURED-PS-CHARS /Y/: <Y OR N></pre> <p>This makes it possible to write PostScript characters in white contoured status.</p> <pre>PLOT REMOTE EXPONENT(S) /Y/: <Y OR N></pre> <p>This sets (Y) or removes (N) the plotting of the remote exponent on the axis.</p> <pre>PLOT SYMBOLS AT NODE POINTS /0/: <#></pre> <p>This makes it possible to plot symbols at the node points on plotted lines on a diagram.</p> <pre>SYMBOL SIZE /.1/: <.#></pre> <p>Set the size of symbols which are plotted at the node points.</p> <pre>WRITE CONDITION? /Y/: <Y OR N></pre> <p>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.</p> <pre>WRITE DATABASE NAME? /Y/: <Y OR N></pre> <p>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.</p> <pre>ALWAYS INITIATE POST ON RE-ENTERING: /Y/: <Y OR N></pre> <p>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.</p> <pre>ALWAYS SOLID LINE: /N/: <Y OR N></pre> <p>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.</p>
--	---

10.30 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 by the SET_PLOT_FORMAT command. 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.

10.31 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.

10.32 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.

10.33 SET_REFERENCE_STATE

The reference state for a component is important when calculating activities, chemical potentials and enthalpies. After a STEP or MAP calculation, 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
Prompt	<p>COMPONENT: <NAME OF THE COMPONENT></p> <p>The name of the component must be given.</p> <p>REFERENCE STATE: <NAME OF A PHASE USED AS THE NEW REFERENCE STATE></p> <p>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.</p> <p>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.</p> <p>TEMPERATURE /*/: <REFERENCE TEMPERATURE></p> <p>Select the temperature (in K) for the reference state. The value * means the current temperature is used for the calculation.</p> <p>PRESSURE /1E5/: <REFERENCE PRESSURE></p> <p>Select the pressure (in Pa) for the reference state. The value * means the current pressure is used for the calculation.</p>

10.34 SET_SCALING_STATUS

When an axis variable is selected by the SET_DIAGRAM_AXIS command, 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
Prompt	<p>AXIS (X, Y OR Z): <NAME OF AN AXIS></p> <p>Specify which axis that you want to set the scaling status.</p> <p>AUTOMATIC SCALING (Y OR N) /N/: <Y OR N></p>

	<p>Choose between automatic (Y) and manual scaling (N). For manual scaling specify these parameters:</p> <p>MIN VALUE: <MINIMUM VALUE></p> <p>The minimum value at the start point of the specified axis.</p> <p>MAX VALUE: <MAXIMUM VALUE></p> <p>The maximum value at the end point of the specified axis.</p>
--	--

10.35 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	<p>TIC TYPE /1/: <1 OR -1 OR 0></p> <p>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.</p>

10.36 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	<p>PLOTTING EVERY TIE-LINE NO /0/: <NUMBER OF TIE-LINES></p> <p>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.</p>

10.37 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.



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. See [ADD_LABEL_TEXT](#) for information.

Syntax	SET_TITLE
Prompt	TITLE: <TITLE>

10.38 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	<p>AXIS (X, Y OR Z): <NAME OF AN AXIS></p> <p>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.</p>


10.39 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 the [RESTORE_PHASE_IN_PLOT](#) command.

Syntax	SUSPEND_PHASE_IN_PLOT
Prompt	<p>PHASE NAME: <NAME OF A PHASE></p> <p>Specify the name of the phase to be suspended from the diagram.</p>

10.40 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 TABULATE command, it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompt	<p>NAME: <NAME OF A TABLE ENTERED IN EITHER POLY OR POST></p> <p>Specify a table name that is entered in either the POLY or POST module.</p> <p>OUTPUT ON SCREEN OR FILE /SCREEN/: <FILE NAME OR RETURN></p> <p>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.</p>

11. Potential, Binary and Ternary Diagram Modules

11.1 POTENTIAL_DIAGRAM Module

The POTENTIAL_DIAGRAM module (short name, the POTENTIAL module) is a simple 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 other commands for this module. Follow the prompts and either search the online help or refer to the [Thermo-Calc User Guide](#) for details about how to calculate using potential diagrams.



Also see Console Mode Example 35.

Syntax	POTENTIAL_DIAGRAM
Prompt	<p>DATABASE: /POT/:</p> <p>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.</p> <p>MATRIX_ELEMENT: /FE/:</p> <p>FIRST_POTENTIAL_SPECIES: /SIO2/:</p> <p>SECOND_POTENTIAL_SPECIES: /O2/:</p> <p>TEMPERATURE: /1000/:</p>

11.2 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) as described in the *Thermo-Calc User Guide*.

Syntax	BINARY_DIAGRAM
Prompt	<p>DATABASE: /TCBIN/:</p> <p>FIRST_ELEMENT:</p> <p>SECOND_ELEMENT</p>

	PHASE DIAGRAM, PHASE FRACTION (F), G- OR A-CURVES (G/A) : /PHASE_DIAGRAM/:
--	---

11.3 TERNARY_DIAGRAM Module

The TERNARY_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple binary 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) as described in the *Thermo-Calc User Guide*.

Syntax	TERNARY_DIAGRAM
Prompt	DATABASE: /FEDEMO/: FIRST ELEMENT: SECOND ELEMENT THIRD ELEMENT PHASE DIAGRAM, MONOVARIENTS, OR LIQUIDUS SURFACE: /PHASE_DIAGRAM/: TEMPERATURE (C) /1000/: GLOBAL MINIMIZATION ON: /Y/:

12. POURBAIX_DIAGRAM Commands

For more information search the online help or see the Pourbaix diagrams educational material and the *Thermo-Calc User Guide* on the [website](#).



Also see examples TCEX40 and TCEX53 for details about using this advanced module.

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 a 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.
- 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 various 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 Fe_{0.93}S 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/:

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:

$$\begin{aligned} \text{Eh} &= \text{MUR}(\text{ZE}) / \text{RNF} \\ \text{pH} &= -\log_{10} [\text{AI}(\text{H}+1, \text{AQUEOUS})] \\ &= -\log_{10} [\text{ACR}(\text{H}+1, \text{AQUEOUS}) * \text{AH}_2\text{O}] \end{aligned}$$

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:

$$\begin{aligned} ML &= Y(AQUEOUS, I) * AH_{2O} / YH_{2O} \\ RC &= ACR(I, AQUEOUS) * YH_{2O} / Y(AQUEOUS, I) \\ AI &= RC * ML \\ &= ACR(I, AQUEOUS) * AH_{2O} \end{aligned}$$

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/:
```

13. REACTOR_SIMULATOR_3 Commands

- [CREATE_DIVIDERS](#)
- [CREATE_PIPES](#)
- [CREATE_STAGE_BOXES](#)
- [EXECUTE_POLY3_COMMAND](#)
- [LIST_RECORDS](#)
- [READ_WORKSPACE](#)
- [SAVE_WORKSPACE](#)
- [START_SIMULATION](#)

13.1 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
Prompt	<p>NUMBER OF DIVIDERS /4/: <THE NUMBER OF DIVIDERS></p> <p>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.</p> <p>NUMBER OF OUTPUTS FOR DIVIDER # /3/: <THE NUMBER OF OUTPUTS></p> <p>Specify the number of outputs for a specific divider #.</p> <p>PERCENT OF INPUT TO OUTPUT 1 /100/: <PERCENT OF INPUT></p> <p>Define the percentage of input to the output 1 in the current divider #.</p> <p>PERCENT OF INPUT TO OUTPUT ## /100/: <PERCENT(S) OF INPUT(S)></p> <p>Define the percentages of inputs to the outputs ## in the current divider #. It is repeated till the last output is specified.</p>

13.2 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
Prompt	<p>FROM RECORD: <A RECORD NUMBER></p> <p>Specify a record number. If there are four segments in the reactor, these records are available:</p> <ul style="list-style-type: none"> • 0 surroundings • 1-4 stage boxes (segments)

	<ul style="list-style-type: none"> • 5–9 dividers (segment boundaries) <p>PIPE TO RECORD: <ANOTHER RECORD NUMBER></p> <p>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 repeated for all inputs and/or outputs for mass and/or heat in current record.</p>
--	---

13.3 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
Prompt	<p>NUMBER OF STAGE BOXES /4/: <THE NUMBER OF STAGE BOXES></p> <p>Specify the number of stage boxes in the reactor. Then define the feed of mass and/or energy (from surroundings to) the reactor.</p> <p>GIVE FEED TO SYSTEM: <FEED></p> <p>One feed (of mass or heat) to the reactor must be specified here. Two types of feeds can be used:</p> <ul style="list-style-type: none"> • 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 ensuring prompt). <p>INPUT TEMPERATURE /298.15/: <INPUT TEMPERATURE></p> <p>GIVE FEED TO SYSTEM: <FEED></p> <p>Specify other feeds (mass or energy) to the reactor. Press <Enter> to finish the feed inputs, and then:</p> <p>GIVE FOR STAGE BOX #</p> <p>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.</p> <p>TYPE OF BOX /EQUILIBRIUM/: <TYPE OF BOX></p> <p>Only the EQUILIBRIUM type is allowed. Press <Enter> to accept it.</p> <p>IS THE STAGE HEAT CONTROLLED? /Y/: <YES OR NO></p> <p>Y means the current segment is heat controlled.</p>

	<p>INITIAL GUESS OF TEMPERATURE? /1000/: <INITIAL TEMPERATURE></p> <p>Give a guess of initial temperature (in K) for the current segment; press <Enter> to accept the default.</p> <p>GIVE INITIAL AMOUNT: <INITIAL AMOUNT OF MASS OR HEAT></p> <p>The initial amount of mass and/or heat in the current segment can be specified here. Two types of initial amount can be used:</p> <ul style="list-style-type: none"> • 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 ensuring prompt). <p>INPUT TEMPERATURE /298.15/: <INPUT TEMPERATURE></p> <p>GIVE INITIAL AMOUNT: <INITIAL AMOUNT OF MASS OR HEAT></p> <p>Specify initial amount (mass or energy) in the current segment. Press <Enter> to finish the initial amount inputs, and then this message displays:</p> <p>EACH PHASE MAY HAVE A SEPARATE OUTPUT, GIVE THESE</p> <p>Now start to define the output for each phase.</p> <p>PHASE NAME /REST/: <NAME OF PHASE></p> <p>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.</p>
--	---

13.4 EXECUTE_POLY3_COMMAND

To directly use all kinds of POLY commands inside the REACTOR module. Any legal POLY commands can be entered.

Syntax	EXECUTE_POLY3_COMMAND
--------	-----------------------

13.5 LIST_RECORDS

Lists all the already-created records for the reactor (including stage boxes, dividers, pipes, etc.).

Syntax	LIST_RECORDS
--------	--------------

13.6 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 a SAVE_WORKSPACE command. The *.RCT file is not printable.

Syntax	READ_WORKSPACE
Options	<p>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.</p> <p>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.</p>

13.7 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 reactor 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
Options	<p>FILE NAME</p> <p>A file name must be specified. The default extension of the RCT file is .RCT, while or any other extension as required.</p> <p>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 warning 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 can use the SAVE command with an unspecified name (i.e. through SAVE , , , command-sequence) to save the REACTOR (and POLY3/GIBBS) workspaces.</p>

13.8 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
Prompt	<p>MAX NUMBER OF LOOPS /10/: <THE MAX NUMBER OF LOOPS></p> <p>Give the max number of loops. The REACTOR module repeats the reactor simulation until this loop number is reached.</p> <p>OUTPUT TO SCREEN OR FILE /SCREEN/: <FILE NAME OR RETURN></p> <p>Decide on either listing simulation results on the screen (by pressing <Enter>) or saving them on an experimental file (with the default extension .EXP).</p> <p> The conditions in each segment are not saved in the file, only on the screen.</p> <p>OUTPUT VARIABLES /T BP(\$)/: <VARIABLE NAME(S)></p> <p>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.</p>

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

```

14. SCHEIL Commands

Search the online help or see the [Thermo-Calc User Guide](#) for details about how to calculate using Scheil either in Graphical Mode (the Scheil Calculator) or Console Mode (the wizard Scheil module).



If you also have a license for DICTRA, you can import a previously calculated Scheil segregation profile into the software using the DICTRA command INPUT_SCHEIL_PROFILE. Search the online help or see the *DICTRA Command Reference* for more information.

- [BCC_TO_FCC_TRANSFORMATION](#)
- [EVALUATE_SEGREGATION_PROFILE](#)
- [GLOBAL_MINIMIZATION](#)
- [LIQUID_PHASE_NAME](#)
- [SAVE_FILE_NAME](#)
- [START_WIZARD](#)
- [STORED_COMPOSITION_TYPE](#)
- [TEMPERATURE_STEP](#)
- [TERMINATION_CRITERIA](#)

14.1 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.

14.2 EVALUATE_SEGREGATION_PROFILE

Use this command for the Scheil module to evaluate the segregation profile.

Syntax	EVALUATE_SEGREGATION_PROFILE
Prompt	EVALUATE SEGREGATION PROFILE? /N/ If answer Y, then note that this feature is not supported with back diffusion: NUMBER OF GRID POINTS /100/ In interactive mode (the command line), a file dialogue window opens. Navigate to the file containing the Scheil profile. Alternately, if you are working from a macro file, the line should contain the name of the file.

14.3 GLOBAL_MINIMIZATION

Use this command for the Scheil module to use global minimization. Also see the POLY commands section about [GLOBAL_MINIMIZATION](#) for more information.

Syntax	GLOBAL_MINIMIZATION
Prompt	<p>USE GLOBAL MINIMIZATION? /N/</p> <p>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.</p>

14.4 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	<p>LIQUID PHASE NAME /DEFAULT/</p> <p>Default selects the liquid phase from the database definitions, otherwise enter a phase name.</p>

14.5 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.

14.6 START_WIZARD

Use this command for the Scheil module to use the wizard with step-by-step prompts to create a Scheil simulation.

Syntax	START_WIZARD
Prompt	<p>DATABASE /TCFE8/:</p> <p>MAJOR ELEMENT OR ALLOY:</p> <p>COMPOSITION INPUT IN MASS (WEIGHT) PERCENT? /Y/:</p> <p>1ST ALLOYING ELEMENT:CR 10 C 1</p> <p>NEXT ALLOYING ELEMENT:</p>

	TEMPERATURE (C) /2000/: FAST DIFFUSING COMPONENTS: /NONE/:C SHOULD ANY PHASE HAVE A MISCIBILITY GAP CHECK? /N/:
--	--

14.7 STORED_COMPOSITION_TYPE

Use this command for the Scheil module to choose the type of composition data to store at the end of a calculation.

Syntax	STORED_COMPOSITION_TYPE
Prompt	TYPE OF COMPOSITION STORED FOR POST PROCESSING: SEGREGATED OR AVERAGE (S/A) The results of a Scheil Calculator activity are stored in the same workspace as the standard POLY-3 calculations. There are two composition data types, <i>segregated</i> (S) or <i>average</i> (A) that can be stored in the workspace. By default, the data are stored in the workspace as a <i>Segregated composition</i> . Choose instead to save the data as an <i>Average composition</i> so you can maintain the mass balance and evaluate several other quantities during a simulation.

14.8 TEMPERATURE_STEP

Use this command for the Scheil module to define a temperature step.

Syntax	TEMPERATURE_STEP
Prompt	SET TEMPERATURE STEP (C) /1/

14.9 TERMINATION_CRITERIA

Use this command for the Scheil module to define the termination criteria for the fraction of liquid or temperature.

Syntax	TERMINATION_CRITERIA
Prompt	FRACTION OF LIQUID OR TEMPERATURE (F OR T)? /F/ FRACTION OF LIQUID /.01/:

15. SYSTEM_UTILITIES Commands

- [ABOUT](#)
- [CLOSE_FILE](#)
- [DISPLAY_LICENSE_INFO](#)
- [HP_CALCULATOR](#)
- [OPEN_FILE](#)
- [SET_COMMAND_UNITS](#)
- [SET_ECHO](#)
- [SET_INTERACTIVE_MODE](#)
- [SET_LOG_FILE](#)
- [SET_PLOT_ENVIRONMENT](#)
- [SET_TC_OPTIONS](#)
- [STOP_ON_ERROR](#)

15.1 ABOUT

Lists basic information about the development history and ownership of the Thermo-Calc and DICTRA software.

Syntax	ABOUT
--------	-------

15.2 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.

15.3 DISPLAY_LICENSE_INFO

Uses a license diagnostics program implemented in the SYS module to detect the license information for the Thermo-Calc installations on the current client computer (and on the connected license server), and lists out all the details of such license information, 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. Also see the [Thermo-Calc Installation Guide](#) on the web for more information.

Syntax	DISPLAY_LICENSE_INFO
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: <MYLICENSEINFO.TXT></p> <p>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.</p>

15.4 HP_CALCULATOR

This is the QBA simple interactive calculator using reverse polish notations.

Syntax	HP_CALCULATOR
	<p>All available OPCODEs (HPC codes) are listed below:</p> <p>Use the BACK command to quit the HP_CALCULATOR and go back to the SYS module.</p> <p>Input are numbers, + - * / and ^ and OPCODEs. Use HELP to list OPCODEs. Several numbers and operations can be given on one line. The content of the X register is displayed after each operation.</p> <p>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 *</p>

15.5 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	<p>FILE NAME: <FILE NAME></p> <p>A legal file name must be specified.</p>

15.6 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 by the [OPEN FILE](#) command.



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>

	<p>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.</p> <p>OUTPUT UNIT NUMBER /6/: <OUTPUT UNIT NAME></p> <p>Specify the output unit number returned from an OPEN_FILE command.</p>
--	---

15.7 SET_ECHO

Designed for use within MACRO files of the Thermo-Calc Console Mode (and DICTRA) software. By adding this command at the beginning of a MACRO *.TCM file [or of the primary MACRO file on the top level if any sub-level(s) of MACRO files are used], it is convenient and extremely useful to automatically display on screen the complete details of various commands in all the sequential operations in the Thermo-Calc Console Mode (and DICTRA) software, that are enforced according to the MACRO file(s). When MACRO files are not used, it is irrelevant to apply this command.

Syntax	SET_ECHO
--------	----------

15.8 SET_INTERACTIVE_MODE

Resets the input and output units to the initial values, i.e. keyboard and screen. Add this command as the last command into your MACRO files, so that you are able to interact with the software after executing the MACRO commands.

Syntax	SET_INTERACTIVE_MODE
--------	----------------------

15.9 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).



To run the example MACRO files go to [Thermo-Calc Console Mode Examples](#)).

Syntax	SET_LOG_FILE
--------	--------------

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.

15.10 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
Prompt	<p>DEFAULT PLOTDEVICE NUMBER /DEFAULT NUMBER/: <DEVICE NUMBER></p> <p>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.</p> <p>PSEUDO FILE NAME: <PSEUDO-FILE NAME></p> <p>The name given here is a symbol which can be used to refer to a physical graphics device when asked for graphical output file.</p> <p>PLOTDEVICE NUMBER /1/: <DEVICE NUMBER></p> <p>The number that specifies the type of graphical device.</p> <p>PLOT FILE NAME: <FILE NAME OR PRINTER NAME></p> <p>The name of the graphical device on system level (name of file or printer).</p> <p>Example:</p> <pre>SET_PLOT_ENVIRONMENT 1 lasp 5 a0tr,,</pre> <p>This example sets the default plot device number to 1, and defines an alias named <code>lasp</code> with plot device 5 and connected to a printer named <code>a0tr</code>.</p>

15.11 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
Prompt	<p>USE_GLOBAL_MINIMIZATION /YES/: <Y OR N></p> <p>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.</p>

	<p><code>GLOBAL_TEST_INTERVAL /0/: <AN INTEGER VALUE></code></p> <p>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 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.</p> <p><code>AUTOMATICALLY_ADD_INITIAL_EQUILIBRIA /YES/: <Y OR N></code></p> <p>When the ADD_INITIAL_EQUILIBRIUM command 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</p> <p><code>SET_AXIS_VARIABLE</code></p> <p>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.</p>
--	---

15.12 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. 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.

Syntax	STOP_ON_ERROR
--------	---------------

16. TABULATION_REACTION Commands

- [ENTER_FUNCTION](#)
- [ENTER_REACTION](#)
- [LIST_SUBSTANCES](#)
- [SET_ENERGY_UNIT](#)
- [SET_PLOT_FORMAT](#)
- [SWITCH_DATABASE](#)
- [TABULATE_DERIVATIVES](#)
- [TABULATE_REACTION](#)
- [TABULATE_SUBSTANCE](#)

16.1 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.

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.

Syntax	ENTER_FUNCTION
Prompt	NAME: <NAME> FUNCTION: <DEFINITION>
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

```

16.2 ENTER_REACTION

This is the same as [TABULATE_REACTION](#) 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 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 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
Prompt	<p>SAME REACTION? /Y/: <Y OR N></p> <p>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.</p> <p>REACTION: <CHEMICAL REACTION EQUATION> & <RA+RB=PC+PD></p> <p>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.:</p> <pre> 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> </pre> <p>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.</p> <p>If typing a file name, the table is displayed and saved as an *.EXP or an *.TAB file. Then prompts:</p> <p>GRAPHICAL OUTPUT /Y/: <Y OR N></p> <p>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.</p> <p>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:</p> <p>PLOT COLUMN? /2/: <1 OR 2 OR 3 OR 4 OR 5 OR 6></p>

	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 <code>POST</code> prompt. The <code>POST</code> module (postprocessor) automatically opens, and all types of the <code>POST</code> -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 <code>BACK</code> or <code>EXIT</code> at the <code>POST</code> prompt always takes you back to the <code>TAB</code> module.
--	--

16.3 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 [TABULATE SUBSTANCE](#) command.

Syntax	LIST_SUBSTANCES
Prompt	<p>WITH ELEMENTS /*/ < * OR A SET OF ELEMENTS ></p> <p>The elements building up various species must be specified. The wildcard * means all elements in the current database.</p> <p>If some elements are specified, it also prompts for how to list species with such elements.</p> <p>EXCLUSIVELY WITH THOSE ELEMENTS /Y/: <Y OR N></p> <p>All species (not phases) in the current database are searched. If the answer is <code>Y</code> (the default), no other elements are allowed in searching, except for those specified. If <code>N</code> all species containing at least one of the specified elements are listed.</p>

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:


16.4 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>

16.5 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 the [SET_PLOT_FORMAT](#) command in the POST module, but is identical to the command [SET_PLOT_ENVIRONMENT](#) command in the SYS (system utility) monitor.

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.

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.

16.6 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.

Syntax	SWITCH_DATABASE
Prompt	<p>DATABASE /XYZ/: <NEW DATABASE NAME></p> <p>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:</p> <p>Use one of these databases</p> <p>PURE4 = SGTE Pure Elements Database v4</p> <p>SSUB3 = SGTE Substances Database v3</p> <p>USER = user defined database</p> <p>DATABASE NAME /XYN/: <new database name></p>

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 for substances, and ENTER_REACTION or TABULATE_REACTION for reactions.

When a predefined database or an appropriate USER database is switched on, the DATA command [GET_DATA](#) is automatically executed; therefore, the TAB module immediately displays a message such as below (in this example the PSUB database is 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:
```

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 Thermo-Calc/DICTRA packages.

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.

16.7 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
Prompt	<p>PHASE NAME /XXXX/: <NAME OF THE PHASE></p> <p>Specify the phase name of a pure phase or a solution phase.</p> <p>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.</p> <p>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.</p> <p> The sum of input site fractions must not exceed unity.</p>

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_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
```

Specify the temperature of interest in K.

```
TEMPERATURE /2000/: <TEMPERATURE OF INTEREST, IN K>
```

Specify the pressure of interest in Pa.

```
PRESSURE /100000/: <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
first 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

```

16.8 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 the SWITCH_DATABASE command 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 $\text{Ga}+\text{S}=\text{GaS}$, $5\text{Al}+2\text{Fe}=\text{Al}_5\text{Fe}_2$.
- Under Linux environments, the notation for a chemical formula treats upper and lower cases as the same (such as $\text{ga}+\text{s}=\text{GaS}$, $5\text{Al}+2\text{Fe}=\text{al}_5\text{fe}_2$); but under Windows, the TAB module only accepts upper cases, e.g. $\text{GA}+\text{S}=\text{GAS}$, $5\text{AL}+2\text{FE}=\text{AL}_5\text{FE}_2$.
- 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 Al_5Fe_2 {e.g. the Al and Fe (but not Al_5Fe_2) may be defined as species, and the Al_5Fe_2 phase may be defined as a two-sublattice stoichiometric phase $[\text{Al}]_5[\text{Fe}]_2$, rather than a single sublattice stoichiometric phase $[\text{Al}_5\text{Fe}_2]$ }, then the reaction $5\text{Al}+2\text{Fe}=\text{Al}_5\text{Fe}_2$ 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 GAL_5FE_2 for 1/7 of the Al_5Fe_2 formula, then the relation $\text{G}(\text{Al}_5\text{Fe}_2)=7*\text{GAL}_5\text{FE}_2$ must be defined; otherwise, the tabulated thermodynamic properties for the reaction $5\text{Al}+2\text{Fe}=\text{Al}_5\text{Fe}_2$ is wrong.

Syntax	TABULATE_REACTION
Prompt	<p>SAME REACTION? /Y/: <Y OR N></p> <p>This prompt displays if there is at least one reaction already defined either by the command ENTER_REACTION or TABULATE_REACTION. If you answer Y, then the next prompt is not asked.</p> <p>REACTION: <CHEMICAL REACTION EQUATION> & <RA+RB=PC+PD></p> <p>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.</p> <p>Pressure /100000/: <pressure of interest, in pa></p> <p>Low temperature limit /298.15/: <T-low, in K> Specify the starting temperature K.</p> <p>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.</p> <p>OUTPUT FILE /SCREEN/: <RETURN FOR SCREEN, OR TYPE A FILE NAME></p> <p>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.</p>

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.



For more information about DATAPLOT search the online help or refer to the *DATAPLOT User Guide* on the website.

Example Output

For the reaction $\text{Ga} + \text{S} = \text{GaS}$ (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

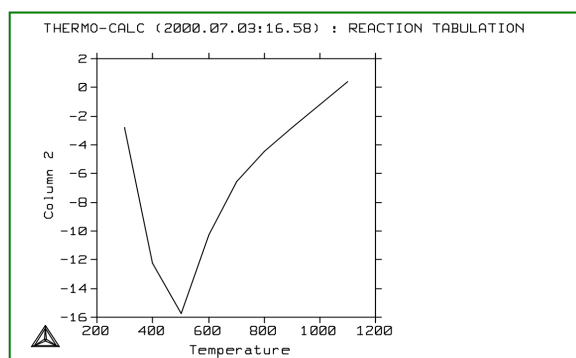
```

```

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

```

Temperature range exceeded for GAlS1




The graph resulted from the TAB module, showing the relation between the heat capacity change (ΔC_p , i.e., column 2 on the resulted table) and temperature (K) for the reaction $\text{Ga} + \text{S} = \text{GaS}$ (data retrieved from the SSUB database). The graph can be refined in the POST Module.

16.9 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	<p>SUBSTANCE (PHASE) : <NAME OF THE SPECIES OR PHASE></p> <p>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 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.</p> <p> 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.</p> <p>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.</p> <p>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.</p> <p>For a pure stoichiometric phase defined with one single sublattice (such as Fe-S, Wustite, and Fe₂O₃-Hematite), no further composition definition is needed.</p> <p>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.</p>

i 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 inter-metallic 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 inter-metallic 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
```

```
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.

	<p>STEP IN TEMPERATURE /100/: <T-STEP> SPECIFY THE TEMPERATURE STEP FOR THE TABULATION.</p> <p>OUTPUT FILE /SCREEN/: <RETURN FOR SCREEN, OR TYPE A FILE NAME></p> <p>If you type <code>Return for screen</code> 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.</p> <p>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:</p> <p>GRAPHICAL OUTPUT /Y/: <Y OR N></p> <ul style="list-style-type: none"> • For <code>N</code> 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 <code>Y</code> 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: <p>PLOT COLUMN ? /2/: <1 OR 2 OR 3 OR 4 OR 5 OR 6></p> <p>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.</p> <p> For more information about DATAPLOT search the online help or refer to the <i>DATAPLOT User Guide</i> on the website.</p>
--	---

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

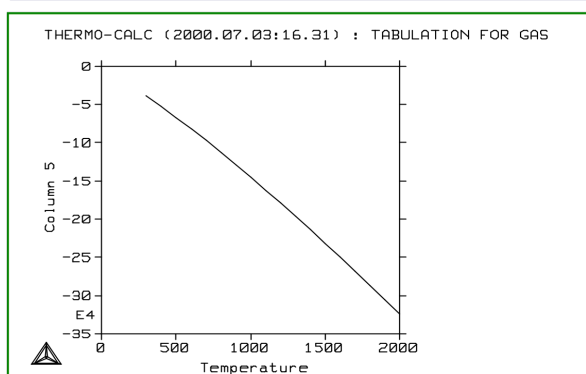
 For a phase, as either an end-member or real solution, the listed species name is irrelevant.

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

TAB:



The graph resulted from the TAB module, showing the relation between Gibbs energy (*i.e.*, column 5 on the resulted table) and temperature (K) for the pure substance H2 (data retrieved from the SSUB database). The graph can be refined in the POST Module.

17. Thermodynamic Variables and Units

The following is about different thermodynamic variables recognised by Thermo-Calc. The sections 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 in the [Thermo-Calc Console Mode Examples](#) to learn about using variables and functions.

- [Thermodynamic Variables](#)
- [Derived Variables and Partial Derivatives](#)
- [Units of State Variables and Derived Variables](#)

17.1 Thermodynamic Variables

There are different thermodynamic variables in Thermo-Calc. Some are *state variables* such as 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_COMPONENT).

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 variables 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 INFORMATION command, 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).

17.1.1 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/size of components in 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 change the value of the variable. This is indicated by putting the R in parenthesis.

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
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.

V	Abbrev.	Unit	Descript.	Domain	Suffix
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 ($\ln AC = MU/RT$)					

Energy-Related Extensive Variables for Whole System or for a Phase

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
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) ¹			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.					

V	Abbrev.	Unit	Descript.	Domain	Suffix
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/size of components in whole system, or amount of a component in system or in a phase.

For NP(ph) or BP(ph), these cannot be used 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)	

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
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
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
<p>1 Do not use in the POLY module.</p> <p>2 Only available in TQ-Interface and TC-API.</p>						

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)

V	Abbrev.	Unit	Descript.	Domain	Suffix
Mb	BMAG(ph) ³	N/A	Bohr magneton number	Phase	R Under a condition and system definition, BMAGR(ph) = BMAG(ph)
<p>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.</p> <p>2 Calculated for phases with magnetic contributions in an equilibrium state. Cannot be used as a condition, but can be plotted in POST.</p> <p>3 Calculated for phases with magnetic contributions in an equilibrium state.</p>					

17.1.2 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 u_i 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 the substitutional matrix element and all substitutional alloying element 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.

17.1.3 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, W, V and F. 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). $GM = \partial G / \partial N$
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). $GW = \partial G / \partial B$
V (per volume in m3)	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). $GV = \partial G / \partial V$

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 is Gibbs energy of the phase per mole of the phase (J/mol). $GM(ph) = \partial G(ph) / \partial NP(ph)$
W (per mass in gram)	First derivative of the variable with regard to the phase amount in terms of BP(ph).	GW is Gibbs energy of the phase per mass of the phase (J/mol). $GW(ph) = \partial G(ph) / \partial BP(ph)$
V (per volume in m3)	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 is Gibbs energy of the phase per volume of the phase (J/mol). $GV(ph) = \partial G(ph) / \partial VP(ph)$
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). $GF(ph) = \partial G(ph) / \partial NP(ph) * NA$

DG(ph) of a Phase

Suffix	Description	Example(s)
M (per mole)	<p>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.</p> <p>DGM(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p>	<p>DGM(ph) is driving force for precipitation of the phase per mole of components.</p> $DGM(ph) = \partial DG(ph) / \partial NP(ph)$
W (per mass in gram)	<p>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.</p> <p>DGW(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p>	<p>DGW(ph) is driving force for precipitation of the phase per mass of components.</p> $DGW(ph) = \partial DG(ph) / \partial BP(ph)$
V (per volume in m3)	<p>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.</p> <p>DGV(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p>	<p>DGV(ph) is driving force for precipitation of the phase per volume of components.</p> $DGV(ph) = \partial DG(ph) / \partial VP(ph)$
F (per mole formula unit)	<p>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.</p>	<p>DGF(ph) is driving force for precipitation of the phase per formula unit of components.</p> $DGF(ph) = \partial DG(ph) / \partial NP(ph) * NA$

Suffix	Description	Example(s)
	DGF(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	

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). $BM = \partial B / \partial N$
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). $NW = \partial N / \partial B$
V (per volume in m3)	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/m3). $NV = \partial N / \partial V$

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(c) cannot be set as a condition.	NM(comp) is mole number of a component per mole of the system (mole fraction, that is, X(comp)). $NM(comp) = \partial N(comp) / \partial N$
W (per mass in gram)	First derivative of the variable with regard to the total system size in terms of B. NW(c) cannot be set as a condition.	BW(comp) is mass (gram) of a component per mass of the system (mass fraction, that is, W(comp)). $BW(comp) = \partial B(comp) / \partial B$
V (per volume in m3)	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). $NV(comp) = \partial N(comp) / \partial V$

NP(ph), BP(ph) and VP(ph) of a Phase in the System

Suffix	Description	Example(s)
M (per mole)	<p>BPM(ph) and VPM(ph): First derivative of the variable with regard to the phase amount in terms of NP(ph).</p> <p>NPM(ph): First derivative of the variable with regard to the total system size in terms of N.</p>	<p>BPM(ph) is mass (gram) of a phase per mole of the phase in the system (g/mol).</p> $\text{BPM(ph)} = \partial \text{BP(ph)} / \partial \text{NP(ph)}$ <p>NPM(ph) is mole number of a phase per mole of the system (mole fraction).</p> $\text{NPM(ph)} = \partial \text{NP(ph)} / \partial N$
W (per mass in gram)	<p>NPW(ph) and VPW(ph): First derivative of the variable with regard to the phase amount in terms of BP(ph).</p> <p>BPW(ph): First derivative of the variable with regard to the total system size in terms of B.</p>	<p>VPW(ph) is volume (m3) of a phase per mass of the phase in the system (m3/g)</p> $\text{VPW(ph)} = \partial \text{VP(ph)} / \partial \text{BP(ph)}$ <p>BPW(ph) is mass (gram) of a phase per mass of the system (mass fraction)</p> $\text{BPW(ph)} = \partial \text{BP(ph)} / \partial B$
V (per volume in m3)	<p>NPV(ph) and BPV(ph): First derivative of the variable with regard to the phase amount in terms of VP(ph).</p> <p>VPV(ph): First derivative of the variable with regard to the total system size in terms of V.</p>	<p>NPV(ph) is mole number of a phase per volume of the phase in the system (mol/m3).</p> $\text{NPV(ph)} = \partial \text{NP(ph)} / \partial \text{VP(ph)}$ <p>VPV(ph) is volume (m3) of a phase per volume of the system (volume fraction).</p> $\text{VPV(ph)} = \partial \text{VP(ph)} / \partial V$


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.	<p>NM(ph,comp) is mole number of a component per mole of a phase (mole fraction of a component in a phase, that is, X(ph, comp)).</p> $\text{NM(ph,comp)} = \partial \text{N(ph,comp)} / \partial \text{NP(ph)}$
W (per mass in gram)	First derivative of the variable with regard to the phase amount in terms of BP(ph) of the phase.	<p>BW(ph,comp) is mass (gram) of a component per mass of a phase (mass fraction of a component in a phase, that is, W(ph, comp)).</p> $\text{BW(ph,comp)} = \partial \text{B(ph,comp)} / \partial \text{BP(ph)}$

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/m ³). $NV(ph,comp) = \frac{\partial N(ph,comp)}{\partial VP(ph)}$

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 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 $LNACR(sp,ph) = LNAC(sp,ph)$.

17.2 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. The following table shows some examples:

Derived variable	Description
$HM.T = \partial HM / \partial T$	Heat capacity for the system at either constant P if pressure is a condition or constant V if volume is a condition.
$HM(ph).T = \partial HM(ph) / \partial T$	Heat capacity for a phase at either constant P if pressure is a condition or constant V if volume is a condition.
$H.T = \partial H / \partial T$	Heat capacity for the system multiplied by total mole number of components, i.e., $\partial H / \partial T = C_p * N$ if pressure is a condition in a closed system or $\partial H / \partial T = C_v * N$ if volume is a condition in a closed system.
$H(ph).T = \partial H(ph) / \partial T$	Heat capacity for a phase multiplied by the sum of NP(ph) and $HM(ph) * \partial NP(ph) / \partial T$, i.e., $C_p(ph) * NP(ph) + HM(ph) * \partial NP(ph) / \partial T$ if pressure is a condition or $C_v(ph) * NP(ph) + HM(ph) * \partial NP(ph) / \partial T$ if volume is a condition.
$VM.T = \partial VM / \partial T$	Thermal expansivity of the system (already multiplied by the total molar volume), i.e., $\partial VM / \partial T = \alpha * VM$.
$VM(ph).T = \partial VM(ph) / \partial T$	Thermal expansivity of a phase (already multiplied by its molar volume), i.e., $\partial VM(ph) / \partial T = \alpha(ph) * VM(ph)$.
$V.T = \partial V / \partial T$	Thermal expansivity of the system (already multiplied by the total volume), i.e., $\partial V / \partial T = \alpha * V$.
$V(ph).T = \partial V(ph) / \partial T$	Thermal expansivity of a phase (already multiplied by the phase volume) plus the $VM(ph) * \partial NP(ph) / \partial T$ term, i.e., $\partial V(ph) / \partial T = \alpha(ph) * V(ph) = \alpha(ph) * VM(ph) * NP(ph) + VM(ph) * \partial NP(ph) / \partial T$.
$VM.P = -\partial VM / \partial P$	Isothermal compressibility of the system (already multiplied by the total molar volume), i.e., $\partial VM / \partial P = -\kappa * VM$.
$VM(ph).P = -\partial VM(ph) / \partial P$	Isothermal compressibility of a phase (already multiplied by its molar volume), i.e., $\partial VM(ph) / \partial P = -\kappa(ph) * VM(ph)$.
$V.P = -\partial V / \partial P$	Isothermal compressibility of the system (already multiplied by the total volume), i.e., $\partial V / \partial P = -\kappa * V$.
$V(ph).P = -\partial V(ph) / \partial P$	Isothermal compressibility of a phase (already multiplied by the phase volume) plus the $VM(ph) * \partial NP(ph) / \partial P$ term, i.e., $\partial V(ph) / \partial P = -\kappa(ph) * V(ph) = -\kappa(ph) * VM(ph) * NP(ph) + VM(ph) * \partial NP(ph) / \partial P$.

Derived variable	Description
$T.X(\text{comp}) = \partial T / \partial X(\text{comp})$	Slope of a phase boundary on a T-X(comp) phase diagram with respect to mole fraction of the component in the system.
$T.W(\text{comp}) = \partial T / \partial W(\text{comp})$	Slope of a phase boundary on a T-W(comp) phase diagram with respect to mass of the component in the system.
$T.X(\text{ph}, \text{comp}) = \partial T / \partial X(\text{ph}, \text{comp})$	Slope of a phase boundary on a T-X(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
$T.W(\text{ph}, \text{comp}) = \partial T / \partial W(\text{ph}, \text{comp})$	Slope of a phase boundary on a T-W(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
$P.T = \partial P / \partial T$	Slope of a phase boundary on a P-T phase diagram (Note that the equilibrium with phase assemblage must be calculated first).

17.2.1 Defining New Derived Variables and Functions

You can define additional derived variables or functions based on a state variable by using the ENTER_SYMBOL command. 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 the following: 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 the EVALUATE_FUNCTIONS command.

17.2.2 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 table. Some derived variables for a gaseous mixture phase are also listed in the table. 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 $\text{pH} = -\log_{10}(\text{AC}(\text{H}^+)) = -\log_{10}(\text{ACR}(\text{H}^+, \text{AQ}))$
Eh	EH	V, mV	Hypothetical electric potential	of the aqueous solution phase $\text{Eh} = u(\text{ZE})/96485.309$
Pe	PE	N/A	Logarithm of the hypothetical electron activity	of the aqueous solution phase $\text{pe} = u(\text{ZE})/(2.3025851 \cdot \text{RT})$
Ah	AH	kJ, kcal	Thermodynamic affinity per electron	of a redox couple wrt the standard hydrogen electrode in the aqueous solution phase $\text{Ah} = u(\text{ZE})$
yw	YH2O	N/A	Mole fraction	of the solvent H2O in the aqueous solution phase $\text{YH2O} = \text{Y}(\text{AQ}, \text{H2O})$
Nw	AH2O	mole	Mole number	of 1.0 kg of solvent H2O $\text{AH2O} = 55.508435$
Nsp	NSH2O	mole	Mole number, $\text{NS}(\text{AQ}, \text{H2O})$	of the solvent (H2O) in the aqueous solution phase $\text{NS}(\text{AQ}, \text{H2O}) = \text{YH2O} \cdot \text{NP}(\text{AQ})$
	NS#		Mole number, $\text{NS}(\text{AQ}, \text{sp})$	of a solute species in the aqueous solution phase $\text{NS}(\text{AQ}, \text{sp}) = \text{Y}(\text{AQ}, \text{sp}) \cdot \text{NP}(\text{AQ})$
M	ML#	mol/kg_H2O	Molality, $\text{ML}(\text{AQ}, \text{sp})$	of a solute species in the aqueous phase $\text{ML}(\text{AQ}, \text{sp}) = \text{Y}(\text{AQ}, \text{sp}) \cdot \text{AH2O} / \text{YH2O}$
m*	TIM	equivalent molality	Total molality	of all solute species in the aqueous solution phase $\text{TIM} = \text{sum}[\text{ML}(\text{AQ}, \text{sp})]\text{ions} + \text{sum}[\text{ML}(\text{AQ}, \text{sp})]\text{complexes}$

Name	Abbrev.	Units	Description	Comments
mt	TIC#	equivalent molality	Total ionic concentration, TIC(AQ,sp)	of a cation I in the aqueous phase $TIC(AQ,spI) = \sum [ML(AQ,spJ) * V(spI - spJ)]$
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 $RC(sp,AQ) = ACR(sp,AQ)/Y(AQ,sp) * YH2O$
α_i	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, $LogAI(H2O,AQ) = \log_{10}[AI(H2O,AQ)]$ $LogAI(sp,AQ) = \log_{10}[AI(sp,AQ)]$
α_w	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 $OS = -55.508435 * \ln AW / TIM$
At1	AT1	equil_mol/kg_H2O	Titration alkalinity (definition 1)	of the aqueous solution phase

Name	Abbrev.	Units	Description	Comments
				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
ft	TFUG	pa, bar, psi	Total gas fugacity	of the gaseous mixture phase TFUG = sum[FUG(sp,GAS)]

17.2.3 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:

$$Pc<name> = X(\text{phase1},\text{component})/X(\text{phase2},\text{component})$$

Another example is the activity coefficient of a component in the system. It is defined as follows:

$$Rc<name> = ACR(\text{component})/X(\text{component})$$

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 Raoult'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:

$$\begin{aligned} RC<spec> &= AI(species,aqueous)/ML(aqueous,species) \\ &= ACR(species,aqueous)/Y(aqueous,species)*Y(aqueous,H2O) \end{aligned}$$

AI is here the activity of solute species calculated from the model, and ML is the molality of the species.

17.2.4 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 examples, 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

17.3 Units of State Variables and Derived Variables

The units for the state variables in the Units column in the table in the section [User-Specified Units](#) 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 section 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 section [Examples of User-Defined Units](#) 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.

17.3.1 User-Specified Units

You do not always need to use the default units for variables. With the ENTER_SYMBOL command, 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 ;
```

See [ENTER_SYMBOL](#) for more information about this command. The following sections are a few examples for entering such conventional functions and the associated units.

17.3.2 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.

 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 = $1.8 * \text{TempC} + 32$	
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)
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

Quantity	Suggested name and expression	Unit
	$Cp3 = HW.T/4.1858$	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	$MU_i = MU(c)/4.1858$	cal/mol
	$MUR_i = MUR(c)/4.1858$	cal/mol
Special quantity for aqueous solution	$pH = -\log_{10}(ACR(H+1))$	dimensionless
	$E_h = MUR(ZE)/RNF$ where $RNF=96485.309$	volts (V)
For extensive variables of a system component		
Amount	$MF_i = N(c)/N = X(c)$	dimensionless
	$MP_i = N(c)/N*100$	dimensionless
	$WF_i = B(c)/B = W(c)$	dimensionless
	$WP_i = B(c)/B*100$	dimensionless
	$BK_{gi} = 1E-3*B(c)$	kilograms (kg)
	$BT_{oni} = 1E-6*B(c)$	tons

Extensive variables of a Phase

Quantity	Suggested name and expression	Unit
Amount	$MF_j = NP(ph)/N$	dimensionless
	$MP_j = NP(ph)/N*100$	dimensionless
	$WF_j = BP(ph)/B$	dimensionless

Quantity	Suggested name and expression	Unit
	$WP_j = BP(ph)/B \cdot 100$	dimensionless
	$BK_{gj} = 1E-3 \cdot BP(ph)$	kilograms (kg)
	$BTon_j = 1E-6 \cdot BP(ph)$	tons
Volume	$VCM_j = 1E-3 \cdot V(ph)$	cubic decimeters (dm ³ , l)
	$VCM_j = 1E-6 \cdot V(ph)$	cubic centimeters (cm ³)
	$VMM_j = 1E-9 \cdot V(ph)$	cubic millimeters (mm ³)
Energy	$GCal_j = G(ph)/4.1858$	cal
	$ACal_j = A(ph)/4.1858$	cal
	$UCal_j = U(ph)/4.1858$	cal
	$HCal_j = H(ph)/4.1858$	cal
	$SCal_j = S(ph)/4.1858$	Cal/K
Driving Force	$DG2_j = DGM(ph)/4.1858$	cal/mol
	$DG3_j = DGW(ph)/4.1858$	cal/g
	$DG4_j = DGV(ph)/4.1858$	Cal/m ³
	$DG5_j = DGF(ph)/4.1858$	cal/mole_formula_unit
Heat Capacity	$Cp2_j = HM(ph) \cdot T/4.1858$	cal/mol/K
	$Cp3_j = HW(ph) \cdot T/4.1858$	cal/g/K
	$Cp4_j = HV(ph) \cdot T/4.1858$	cal/m ³ /K
	$Cp5_j = HF(ph) \cdot T/4.1858$	cal/mole_formula_unit/K
Thermal Expansion	$A2_j = VM(ph) \cdot T \cdot 1E-6 \cdot VM$	cm ³ /mol/K
	$A3_j = VW(ph) \cdot T \cdot 1E-6 \cdot VM$	cm ³ /g/K
	$A4_j = VF(ph) \cdot T \cdot 1E-6 \cdot VM$	cm ³ /mole_formula_unit/K
Isothermal Compressibility	$B2_j = -VM(ph) \cdot P \cdot 1E-9 \cdot VM$	mm ³ /mol/Pa
	$B3_j = -VW(ph) \cdot P \cdot 1E-9 \cdot VM$	mm ³ /g/Pa
	$B4_j = -VF(ph) \cdot P \cdot 1E-9 \cdot VM$	mm ³ /mole_formula_unit/Pa

Extensive variables of a Component in a Phase

Quantity	Suggested name and expression	Unit
Amount	$MF_{ij} = N(ph,c)/NP(ph) = X(ph,c)$	dimensionless
	$MP_{ij} = N(ph,c)/NP(ph)*100$	dimensionless
	$WF_{ij} = B(ph,c)/BP(ph) = W(ph,c)$	dimensionless
	$WP_{ij} = B(ph,c)/BP(ph)*100$	dimensionless
	$BKg_{ij} = 1E-3*B(ph,c)$	kilograms (kg)
	$BTon_{ij} = 1E-6*B(ph,c)$	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	$MUCal_{ij} = MU(sp,ph)/4.1858$	cal/mol
	$MUErg_{ij} = MU(sp,ph)*1E7$	cal/mol
Fugacity	$FA_{ij} = AC(sp,ph)*PATM$	atmosphere (atm)
	$FB_{ij} = AC(sp,ph)*PB$	bars (bar)
	$FC_{ij} = AC(sp,ph)*PKB$	kilobars (kbar)
	$FT_{ij} = AC(sp,ph)*PTOR$	Tors (millimeters of Hg)
ln(Fugacity)	$LnFA_{ij} = LNAC(sp,ph)+LN(PATM)$	atmosphere (atm)
	$LnFB_{ij} = LNAC(sp,ph)+LN(PB)$	bars (bar)
	$LnFC_{ij} = LNAC(sp,ph)+LN(PKB)$	kilobars (kbar)
	$LnFT_{ij} = LNAC(sp,ph)+LN(PTOR)$	Tors (millimeters of Hg)
Special quantity for aqueous solution	$Alij=ACR(Fe+3,AQ)*AH2O$	dimensionless
	$RCij=ACR(Fe+3,AQ)*YH2O/Y(AQ,Fe+3)$ where $AH2O=55.508435$ and $YH2O=Y(AQ,H2O)$	dimensionless

Quantity	Suggested name and expression	Unit
	$WRC_{lij} = WR(AQ,sp)/4.1858$ (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	$ML_{ij} = Y(AQ, FE+3) \cdot AH_{2O} / YH_{2O}$	molality (m)
	$ISTR = 1 \cdot IS_1 + 1 \cdot IS_2 + 1 \cdot IS_3$ where $AH_{2O} = 55.508435$, $YH_{2O} = Y(AQ, H_2O)$ and $IS_n = .5 \cdot ML_i \cdot Z_i^{**2} + .5 \cdot ML_j \cdot Z_j^{**2} + .5 \cdot ML_k \cdot Z_k^{**2}$	molality (m)

17.3.3 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 i th -order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
$TC(ph,sp)$ $TC(ph,sp;0)$	Curie temperature (K) of a pure substance or end-member.

Variables	Description and unit
TC(ph,sp1;sp2;...;0)	
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.
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 (m3) 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 (m3) 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 (m3) 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 (m3/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 (m3/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.