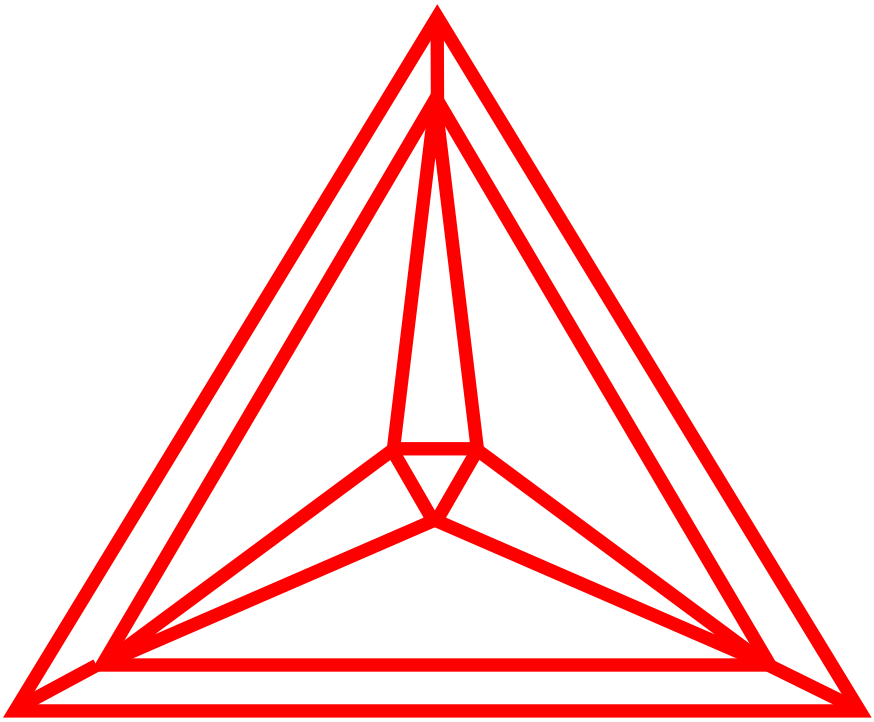
Thermo-Calc®

Examples

Version S



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Stockholm, Sweden

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There may be some minor differences in contents between this Examples Book and the actual appearance of the program (as seen on the screen when running the Thermo-Calc Classic version S). This is because that some of the contents may need to be updated along with the continuous development of the program. Please visit the Thermo-Calc Software web site (www.thermocalc.com) for any modification and/or improvement that have been incorporated into the program and its on-line help, or any amendment that have made to the content of the User's Guides and to the FAQ lists and other technical information publications.

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Thermo-Calc Examples

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Introduction

The examples in this volume give an idea of how to operate the Thermo-Calc system on line. Many of the different databases are used and the normal amount of erroneous input is included in the examples. Some examples have a direct applicaiton but most are just designed to show features of Thermo-Calc.

The typography of this volume is worth noting. As the use of Thermo-Calc is interactive it is important to distinguish clearly the user input from the output of the program. In all examples the computer output is writtne with `the Courier font`. User input is written with **`a larger font and in bold`**. Comments are in ***`bold-oblique but with a smaller size`***. Finally, as the commands in Thermo-Calc are usually abbreviated the command in full is usually echoed on the following line written in *`italics`*.

Note

Due to the growing number of examples some of those that are listed in the content may have not been included due to lack of space. If some of the missing would be of particular interest to you please contact support@thermocalc.se.

Revision history

October 1988	First release
May 1990	Complete revision to POLY-3
January 1991	Revision for version G
June 1993	Revision for version J
January 1998	Revision for version L
April 1999	Revision for version M
September 2001	Revision for version N
November 2002	Revision for version P
May 2004	Revision for version Q
September 2006	Revision for version R
June 2008	Revision for version S

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33. Benchmark calculation - An isopleth in the Fe-Cr-C system.
34. Calculation of the phase diagram and G curves in the Al-Zn system.
35. Calculation of potential diagram.
36. Assessment - The use of the PARROT module.
37. Calculation of an isothermal section using command lines.
38. Calculation of the Morral "rose".
39. Calculation of the reversible Carnot cycle of a heat engine.
40. POURBAIX module.
41. Calculation of a solubility product.
42. Formation of Para-pearlite (Isopleth calculation).
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44. Exploring the usage of variables and functions.

45. 3D-diagram with the gamma volume in the Fe-Cr-C system.
46. 3D-diagram with the liquidus surface of the Fe-Cr-C system.
47. Quarternary diagram with the gamma volume in the Fe-Cr-V-C system at 1373K.
48. Scheil Simulation with Interstitial Back Diffusion.
49. Quasichemical Model via G-E-S.
50. Quasichemical Model via TDB.
51. Calculation of molar volume, thermal expansivity and density.
52. Changing the excess models for interaction parameters in a solution phase.
53. Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine.

1

Calculation of the binary Fe-C phase diagram (Exploring the HELP facilities)

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of the Fe-C binary phase diagram
SYS: @@
SYS: set-log ex01,,,
SYS:
SYS: @@ The log file is set to get command echo.
SYS: @@ The menu is shown by typing a question mark "?"
SYS: ?
   ... the command in full is HELP
 BACK                    INFORMATION             SET_LOG_FILE
 CLOSE_FILE              MACRO_FILE_OPEN         SET_PLOT_ENVIRONMENT
 EXIT                    OPEN_FILE               SET_TC_OPTIONS
 GOTO_MODULE             SET_COMMAND_UNITS       SET_TERMINAL
 HELP                    SET_ECHO                STOP_ON_ERROR
 HP_CALCULATOR           SET_INTERACTIVE_MODE
SYS: @@ When you give a command the program may ask questions.
SYS: @@ You may obtain help for each question by typing a ? .
SYS: @@ If you accept the default answer suggested /within slashes/
SYS: @@ just press "return"
SYS: info
   ... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/:  ?
 WHICH SUBJECT

 Specify a subject (or its abbreviation as long as it is unique, e.g.,
 TCC, TC4A, TCW, TC4U, TAB, TDB, TERN, TC-TOOLBOX, THERMO-CALC ENGINE,
 TQ, TCMI, etc.) on which information should be given, from the following
 subjects that are important to the use of the SYS Module:

  PURPOSE (Introducing the THERMO-CALC Software Package)
  COMPUTATIONAL THERMODYNAMICS
  TCC - THERMO-CALC CLASSIC         TCW - THERMO-CALC WINDOWS
  TC4A - THERMO-CALC FOR ACADEMIC   TC4U - THERMO-CALC FOR UNIVERSITY
  MODELS IN THERMO-CALC             MODULES OF THERMO-CALC
  DATABASES IN THERMO-CALC          FUNCTIONALITY OF THERMO-CALC
  STATE VARIABLES                   INTENSIVE VARIABLES
  EXTENSIVE VARIABLES               DERIVED VARIABLES
  UNITS                             BASIC UNITS
  SYSTEM UNITS                      COMPONENT UNITS
  PHASE UNITS                       PHASE-COMPONENT UNITS
  PHASE-SPECIES UNITS               USER-SPECIFIED UNITS
  PHASE DIAGRAMS                    PROPERTY DIAGRAMS
  TDB (DATABASE RETRIEVAL)          GES (GIBBS_ENERGY_SYSTEM)
  POLY (EQUILIBRIUM CALCULATIONS)   POST (POST_PROCESSOR)
  PARROT (ASSESSMENT)               ED_EXP (EDIT_EXPERIEMENT)
  BIN (BINARY_DIAGRAM)              TERN (TERNARY_DIAGRAM)
  POT (POTENTIAL_DIAGRAM)           POURBAIX (POURBAIX_DIAGRAM)
  TAB (TABULATION)                  CHEMICAL EQUATION
  SCHEIL (SCHEIL_SIMULATION)        REACTOR (REACTOR_SIMULATOR)
  SYS (SYSTEM_UTILITY)              FOP (FUNCTION_OPT_PLOT)
  USER INTERFACE OF THERMO-CALC     GUI (GRAPHICAL USER INTERFACE)
  APPLICATIONS OF THERMO-CALC       THERMO-CALC ENGINE
  API - PROGRAMMING INTERFACE       TQ/TCAPI INTERFACES
  TC-TOOLBOX IN MATLAB SOFTWARE     TCMI MATERIALS INTERFACE
  GLOBAL (Global Minimization Technique in the Thermo-Calc software)
  DICTRA (Diffusion-Controlled Transformation Simulation Software)
  HELP   (How to get on-line help in the TCC software)
  NEWS   (Revision History and New Features of the TCC Software)

WHICH SUBJECT /PURPOSE/:
 PURPOSE

             INTRODUCTION to the System Utility Module (SYS)
          ************************************************

 Thermo-Calc is one of the most powerful and flexible software package
```

in the field of Computational Thermodynamics. It has been widely used for all kinds of thermochemical calculations of complicated heterogeneous phase equilibria and multicomponent phase diagrams. Available for most platforms, the Thermo-Calc software provides you with basic thermodynamic necessities, such as equilibrium calculations, phase and property diagrams, and thermodynamic factors (driving forces) in multicomponent systems.

Thermo-Calc features a wide spectrum of models, making it possible to perform calculations on most complex problems involving thermodynamics.

Thermo-Calc consists of several basic and advanced modules for equilibrium calculations, phase and property diagram calculations, tabulation of thermodynamic quantities, database management, assessment of model parameters, experimental data manipulations, and post-processing of graphical presentations.

Thermo-Calc facilitates a comprehensive data bank of assessed thermochemical data for the phases in various systems, and there are many comprehensive databases covering a very wide range of industrial materials and applications.

Thermo-Calc enables you to establish your own databases through critical assessment based on all kinds of experimental information.

Thermo-Calc utilizes a flexible user interface that is easy to use. Additionally, a complete GUI (graphical user interface) version, i.e., TCW (Thermo-Calc Windows), has been developed.

Thermo-Calc presents the standard thermodynamic calculation engine that has the fastest and most stable mathematical and thermodynamic solutions. Any other software that requires precisely calculated thermochemical quantities can make use of the Thermo-Calc Engine through the TQ and TCAPI programming interfaces.

The advantages of Thermo-Calc are its multiple applications. Several departments or divisions at the same company, institute or university can use the packages for different purposes. Proven application examples include industries such as steel plants, aerospace, transportation, and manufacturing. With the facilities provided by Thermo-Calc, you can optimize your materials processes to produce a higher yield, better product at a lower cost.

The classical versions of both Thermo-Calc and DICTRA software have a so-called System Utility Module (under the SYS prompt), which provides the primary controls on inter-module communication, MACRO-file creation and operation, working and plotting environmental setting, and command information searching. They are essential for properly performing ordinary calculations, desirably obtaining calculated results, and easily conducting various tasks.

It also facilitates some odd features, such as user interface setting, command unit setting, error reporting preference, terminal characteristics definition, workspace listing, open or close of a file through a unit, interactive calculator, news retrieval, etc. Some of such odd commands are used for performance preference of the users, and some are designed for debugging of the programmers. Few odd commands are included only for some special purposes, which might have been obsolete in later versions.

The following commands are available in the SYS module:

```
 SYS:?
  BACK                    HP_CALCULATOR           SET_INTERACTIVE_MODE
  CLOSE_FILE              INFORMATION             SET_LOG_FILE
  EXIT                    MACRO_FILE_OPEN         SET_PLOT_ENVIRONMENT
  GOTO_MODULE             OPEN_FILE               SET_TERMINAL
  HELP                    SET_COMMAND_UNITS       STOP_ON_ERROR
 SYS:
```

Notes for versions since TCCR:

* Five SYS commands have been taken away from the SYS-Module monitor (and also eliminated from this chapter in the TCCR User’s Guide), because they are normally for system debugging purpose only, or obsolete now, or totally irrelevant. Such commands include: NEWS, LIST_FREE_WORKSPACE, PATCH, SET_ERROR_MESSAGE_UNIT and TRACE.
* The Section 14.3 (Display of General Information) has been completely removed from this chapter since the TCCR User’s Guide. However, for

```
      the purpose of obtaining information about various subjects in
      the SYS module, please use the on-line help feature of the TCCR
      software, i.e., typing the INFORMATON <SUBJECT> command sequence
      in the SYS module, that will follow a display on screen of some
      brief information on a certain subject related to the Thermo-Calc
      software/database/interface package.
  * The FOP Module (FUNC_OPT_PLOT, the simple function optimizer and
      plotting facility; for function/parameter mathematic-fitting and
      plotting) has been completely eliminated from the TCCR software.
      One should instead use the PARROT module to perform critical
      thermodynamic assessments.
  * In the meantime, the SYS command SET_ECHO (that has been blindly
      existing in the TCC and DICTRA software for a very long time)
      is documented in the current edition of this chapter in the
      TCCR User's Guide; see Section 14.2.6 and 14.2.8.

 Revision History of the SYS Module User's Guide:
 ================================================
  Mar 1985  First release
                    (Edited by Bo Sundman)
  Oct 1993  Second revised release
                    (Edited by Bo Sundman)
  Sept 1996 Third revised release
                    (Edited by Mikael Schalin and Bo Sundman)
  Jun 2000  Fourth revised and extended release
                    (Edited by Pingfang Shi)
  Nov 2002  Fifth revised release
                    (Edited by Pingfang Shi)
  Jun 2004  Sixth revised and extended release
                    (Edited by Pingfang Shi)
  Aug 2006  Seven revised and simplified release
                    (Edited by Pingfang Shi)

WHICH SUBJECT:
SYS: @?<Hit_return_to_continue>
SYS: @@ For a binary phase diagram calculation we use the binary module
SYS: go
   ... the command in full is GOTO_MODULE
MODULE NAME: ?
 NO SUCH MODULE, USE ANY OF THESE:
 SYSTEM_UTILITIES
 GIBBS_ENERGY_SYSTEM
 TABULATION_REACTION
 POLY_3
 BINARY_DIAGRAM_EASY
 DATABASE_RETRIEVAL
 REACTOR_SIMULATOR_3
 PARROT
 POTENTIAL_DIAGRAM
 SCHEIL_SIMULATION
 POURBAIX_DIAGRAM
 TERNARY_DIAGRAM
MODULE NAME: BIN
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/:  PBIN
 Current database: TCS Public Binary Alloys TDB v1

 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
First element: fe
Second element: c
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:  Phase-Diagram
   ... the command in full is REJECT
 VA                      /-  DEFINED
```

```
IONIC_LIQ:Y             L12_FCC                 B2_BCC
BCC_B2  REJECTED
REINITIATING GES5 .....
  ... the command in full is DEFINE_ELEMENTS
C                       FE  DEFINED
  ... the command in full is GET_DATA
ELEMENTS .....
SPECIES ......
PHASES .......
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

  90Din 'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report
      DMA(A)195, Rev. August 1990'
  85Gus 'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267
      TRITA 0237 (1984); C-FE'
  89Din 'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report
      DMA(A)195, September 1989'
  91Din 'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, Vol.15,
      No.4, pp.317-425, (1991)'
-OK-
  ... the command in full is SET_AXIS_VARIABLE
The condition X(FE)=.1234  created
  ... the command in full is SET_AXIS_VARIABLE
The condition T=1319.08  created
  ... the command in full is SET_REFERENCE_STATE
  ... the command in full is SET_REFERENCE_STATE
  ... the command in full is SAVE_WORKSPACES
Start points provided by database
  ... the command in full is SAVE_WORKSPACES
Version S mapping is selected

Organizing start points

Generating start point   1
Generating start point   2

Phase region boundary   1 at:   4.637E-01  1.319E+03
    FCC_A1
 ** GRAPHITE
*** Buffer saved on file: BINARY.POLY3
Calculated.           14  equilibria

Phase region boundary   2 at:   4.845E-01  1.011E+03
 ** BCC_A2
    FCC_A1
 ** GRAPHITE

Phase region boundary   3 at:   9.841E-01  1.011E+03
 ** BCC_A2
    FCC_A1
Calculated           33  equilibria

Phase region boundary   4 at:   4.996E-01  1.011E+03
 ** BCC_A2
    GRAPHITE
Calculated..          30  equilibria
Terminating at axis limit.

      :
      :
      :

Phase region boundary   9 at:   9.939E-01  1.768E+03
 ** BCC_A2
    FCC_A1
Calculated           18  equilibria
```

```
 Phase region boundary  10 at:   9.858E-01  1.768E+03
    LIQUID
  ** BCC_A2
 Calculated           22  equilibria

 Phase region boundary  11 at:   4.129E-01  1.427E+03
  ** LIQUID
    GRAPHITE
 Calculated..          44  equilibria
 Terminating at axis limit.

 Phase region boundary  12 at:   4.637E-01  1.319E+03
    FCC_A1
  ** GRAPHITE
 Calculated.            6  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: BINARY.POLY3
 CPU time for mapping           0  seconds

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is SET_TIELINE_STATUS
   ... the command in full is SET_LABEL_CURVE_OPTION
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ One can interactively specify an output device as follows. The command
POST: @@ '@#1' asks the user to input a value for the variable #1, which can be used
POST: @@ later on. The default value (input by pressing RETURN) is 9, meaning
POST: @@ output to SCREEN.
POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,
POST:
POST: set-title example 1a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ By default no label is given, the user must specify it himself.
POST: @@ There are two possibilities, to label the lines or to label the
POST: @@ areas. In the latter case the user must supply a coordinate for the
POST: @@ label, for example
POST: ADD
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .1
Give Y coordinate in axis units: 2000
Automatic phase labels? /Y/:  Y
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated          825  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: LIQUID
Text size: /.3999999762/:
POST: set-title example 1b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: add .4 900
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:  Y
 Automatic labelling not always possible
```

```
 Using global minimization procedure
 Calculated          825  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: FCC_A1+GRAPHITE
Text size: /.3999999762/:
POST: set-title example 1c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ This is the stable phase diagram with graphite and no cementite.
POST: @@ In TC all relevant data from the calculation of the diagram is saved
POST: @@ and it is possible to plot the same diagram using other thermodynamic
POST: @@ quantities, for example replace the carbon composition with its activity
POST: @@ Find out the commands in the post processor by inputing ?
POST: ?
   ... the command in full is HELP
 APPEND_EXPERIMENTAL_DATA QUICK_EXPERIMENTAL_PLOT  SET_PLOT_OPTIONS
 BACK                     REINITIATE_PLOT_SETTINGS SET_PLOT_SIZE
 CREATE_3D_PLOTFILE       RESTORE_PHASE_IN_PLOT    SET_PREFIX_SCALING
 DUMP_DIAGRAM             SET_AXIS_LENGTH          SET_RASTER_STATUS
 ENTER_SYMBOL             SET_AXIS_PLOT_STATUS     SET_REFERENCE_STATE
 EXIT                     SET_AXIS_TEXT_STATUS     SET_SCALING_STATUS
 FIND_LINE                SET_AXIS_TYPE            SET_TIC_TYPE
 HELP                     SET_COLOR                SET_TIELINE_STATUS
 LIST_DATA_TABLE          SET_CORNER_TEXT          SET_TITLE
 LIST_PLOT_SETTINGS       SET_DIAGRAM_AXIS         SET_TRUE_MANUAL_SCALING
 LIST_SYMBOLS             SET_DIAGRAM_TYPE         SUSPEND_PHASE_IN_PLOT
 MAKE_EXPERIMENTAL_DATAFI SET_FONT                 TABULATE
 MODIFY_LABEL_TEXT        SET_INTERACTIVE_MODE
 PATCH_WORKSPACE          SET_LABEL_CURVE_OPTION
POST: @@ The command to set axis for the diagram is SET-DIAGRAM-AXIS
POST: s-d-a x
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
 UNKNOWN QUESTION VARIABLE :
VARIABLE : ac
FOR COMPONENT : c
POST: set-title example 1d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ The diagram stops at unit activity which represent graphite.
POST: @@ The labels disappear when one sets a new diagram axis because they
POST: @@ are relative to the axis values, not the axis quantities.
POST: @@
POST: @@ A simpler way to identify the stable phases is to use
POST: @@ the command set-label
POST: set-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/:  ?
 THE OPTIONS MEANS:
 A     LIST STABLE PHASES ALONG LINE
 B     AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
 C     LIST AXIS QUANTITIES
 D     AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
 E     AS B WITH CHANGING COLORS
 F     AS D WITH CHANGING COLORS
 N     NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/:  B
POST: set-title example 1e
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ The metastable diagram, with cementite, can also be calculated but then
```

POST: ***@@ one must do some manipulations in POLY. We can use the data***
POST: ***@@ we already retrieved from the database.***
POST: **back**
 Current database: TCS Steels/Fe-Alloys Database v6

 VA DEFINED
 IONIC_LIQ:Y L12_FCC B2_BCC
 B2_VACANCY HIGH_SIGMA DICTRA_FCC_A1
   REJECTED
SYS: **go p-3**
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: ***@@ The BIN module has used the poly-3 workspace to calculate the***
POLY_3: ***@@ diagram. We have all data available here. The workspace has been***
POLY_3: ***@@ saved on a file and we can read this back with the command READ.***
POLY_3:
POLY_3: **read BINARY**
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: ***@@ There are many command in the POLY module. They make it possible***
POLY_3: ***@@ to calculate almost any kind of equilibrium and diagram.***
POLY_3: ***@@ With the ? we can list all commands***
POLY_3: **?**
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM EXIT REINITIATE_MODULE
 ADVANCED_OPTIONS GOTO_MODULE SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA HELP SELECT_EQUILIBRIUM
 BACK INFORMATION SET_ALL_START_VALUES
 CHANGE_STATUS LIST_AXIS_VARIABLE SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM LIST_CONDITIONS SET_CONDITION
 COMPUTE_TRANSITION LIST_EQUILIBRIUM SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM LIST_INITIAL_EQUILIBRIA SET_INTERACTIVE
 DEFINE_COMPONENTS LIST_STATUS SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM LIST_SYMBOLS SET_REFERENCE_STATE
 DEFINE_MATERIAL LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB MACRO_FILE_OPEN SET_START_VALUE
 DELETE_SYMBOL MAP SHOW_VALUE
 ENTER_SYMBOL POST STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS READ_WORKSPACES TABULATE
POLY_3:
POLY_3: **@?<Hit_return_to_continue>**
POLY_3: ***@@ More information about a command can be obtaind with the HELP command***
POLY_3: **help**
COMMAND: **list-status**
 LIST_STATUS

 The status of components, species or phases can be listed with this command.
 The user may select all or some of these.

 Synopsis 1:   LIST_STATUS <keyword(s)>
 Synopsis 2:   LIST_STATUS
 Ensuing Prompt: Option /CPS/: <keyword(s)>

 Keyword = C   means list component status
           P   means list phase status
           S   means list species status

 Default is CPS. By pressing <RETURN>, a complete list with status for
 components, phases and species is obtained. By just giving P, a list
 of just the phase statuses is obtained. If you are also interested in
 component status, then type C. You may also simply input CS so that
 a list of statuses for both components and species can be listed out.

 The statuses of components, phases and species can be changed with the
 CHANGE_STATUS command.

 Results: Depending upon the key word specified in the CHANGE_STATUS options,
  a table with the current statuses of phases or species or components, or
  their combinations, is shown up.
  * For components, their statuses and reference states are listed.
  * For ENTERED and FIXED phases, their statuses, driving forces and
      equilibrated amount (of stable) are listed. Note that the metastable
      phases are listed in descending order of stability. To avoid long
      outputs, in the versions later than version N, only 10 metastable

```
     phases (in ENTERED status) will be listed by lines, while all other
     less stable phases are merged onto one line. For DORMANT phases,
     their phase names and driving forces are listed. For SUSPENDED phases,
     only the phase names are listed into one line.
 * For species, only the status are listed out.

 Example:
  POLY_3:l-st
  Option /CPS/:
  *** STATUS FOR ALL COMPONENTS
  COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
  VA                      ENTERED   SER
  C                       ENTERED   GRAPHITE       *              *
  FE                      ENTERED   SER
  NI                      ENTERED   SER
  *** STATUS FOR ALL PHASES
  PHASE                   STATUS    DRIVING FORCE   MOLES
  FCC_A1                  FIXED      0.00000000E+00  1.00000000E+00
  BCC_A2                  ENTERED    0.00000000E+00  0.00000000E+00
  HCP_A3                  ENTERED   -2.69336869E-01  0.00000000E+00
  CEMENTITE               ENTERED   -2.86321394E-01  0.00000000E+00
  M23C6                   ENTERED   -3.44809821E-01  0.00000000E+00
  LIQUID                  ENTERED   -4.95421844E-01  0.00000000E+00
  CBCC_A12                ENTERED   -6.16764645E-01  0.00000000E+00
  M7C3                    ENTERED   -6.56332559E-01  0.00000000E+00
  M5C2                    ENTERED   -6.83594326E-01  0.00000000E+00
  GRAPHITE                ENTERED   -1.02142788E+00  0.00000000E+00
  DIAMOND_A4              ENTERED   -1.73225646E+00  0.00000000E+00
  ALNI_B2                 ENTERED   -4.79816887E+00  0.00000000E+00
  ENTERED PHASES WITH DRIVING FORCE LESS THAN    -4.80
  AL3NI2 GAS
  HCP_A3                  DORMANT   -2.69336869E-01
  SUSPENDED PHASES:
  V3C2 KSI_CARBIDE FECN_CHI FE4N CUB_A13
  *** STATUS FOR ALL SPECIES
  C  ENTERED    C2 ENTERED    C4 ENTERED    C6 ENTERED    FE ENTERED
  C1 ENTERED    C3 ENTERED    C5 ENTERED    C7 ENTERED    NI ENTERED
  VA ENTERED

 The statuses of components, phases and species can be changed with the
 CHANGE_STATUS command.

POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ General information can be obtained using the INFORMATION command
POLY_3: INFO
   ... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/:
 PURPOSE

          INTRODUCTION to the Equilibrium Calculation Module (POLY)
         ***********************************************************

 Knowledge of the thermodynamic equilibrium is an important factor for
 understanding properties of materials and processes. With a database of
 thermodynamic model parameters, it is possible to predict such properties
 and also to obtain driving forces for diffusion-controlled phase
 transformations and other dynamic processes.

 With the comprehensive Equilibrium Calculation module, POLY ? it is possible
 to calculate many different kinds of equilibria and diagrams, in particular
 multicomponent phase diagrams. This is thus an important tool in developing
 new materials and processes. The current POLY module is its third version;
 this is why is often referred as POLY_3 in the Thermo-Calc software.

 Different kind of databases can be used with the POLY module, and thus it
 can be used for alloys or ceramic system, as well as gaseous equilibria,
 aqueous solution involved heterogeneous interaction systems. Since TCCN,
 up to 40 elements and 1000 species can be defined into a single system
 (previously 20 elements and 400 species) for equilibrium calculations.

 Great care has been taken to provide the users with the most flexible tool.
 All normal thermodynamic state variables can be used to set as conditions in
 calculating equilibria, and as axes in plotting diagrams. A unique facility
 is to set the composition or any property of an individual phase as a
```

condition. Any state variable can be varied along an axis in order to generate a diagram. During calculations of a diagram, complete descriptions of all calculated equilibria are stored, and in the diagram any state variable can be used as axis.

One of the major improvements since the TCCR/TCW4 software version is that the recently-implemented Global Minimization Technique is used to assure that the present minimum in an equilibrium calculation is the most stable minima for the specified conditions. This new technique, which is based on the traditional GEM (Gibbs Energy Minimization) Technique (i.e., the ordinary POLY Minimization routines used in previous versions, where pre-knowledge of miscibility gaps in involved phases are necessary, otherwise, metastable equilibria instead of the stable equilibria may be obtained), will ultimately prevent a calculation from reaching an undesired metastable or unstable (local) equilibrium in a defined system, and automatically detect possible miscibility gap(s) and automatically create additional composition sets in a solution phase if needed for handling single or multiple miscibility gaps. Therefore it is no longer necessary for the user to specify additional composition sets in advance.

A Direct Global Minimization can be performed on conditions: N, n(comp), B, b(comp), w(comp), x(comp), T, and P, but not when combined conditions as e.g. w(a)-3*w(b)=1 are used or when an activity or potential condition is used. For all other types of conditions where regular minimization converges, Indirect Global Minimization, i.e. global test and corrections, if necessary, are performed until the lowest minimum is found.

 * Direct Global Minimization: From the mesh of Gibbs energy, find the set of grid points that gives the lowest energy solution under the specified conditions. This set of grid points provides starting combination of phases and their constitutions for regular minimization to find the exact equilibrium solution. This solution will be then subject to a global test as described below.

 * Indirect Global Minimization: Under certain conditions, direct approach is impossible. In this case, regular minimization is performed first and then a check is performed in order to see if the found local minimum is a global one by checking if all grid points are above the equilibrium Gibbs energy plane. If not, then recalculate by including these grid points until no grid point is above the equilibrium Gibbs energy plane from the previous step.

The full-scale and full-scope usage of the Global Minimization Technique has been extended from for only single-point calculations within TCCR/TCW4 to for all types of calculations (of single-points, property diagram stepping and phase diagram mapping) within TCCS/TCW5.

The use of Global Minimization Technique may increase the computation time, while it is not an issue at all, thanks for the rapid developments of computer hardware nowadays.

 * The main cost in time comes from the calculation of Gibbs energy at each grid point generated by properly meshing the composition space for each entered phase. In a typical multicomponent system calculation, about 100MB of RAM memory is needed in storing the mesh of Gibbs energies.

 * An additional (but much smaller) cost in time comes from finding the set of grid points in the above mesh that give the lowest energy solution. This solution is where POLY starts its ordinary minimization. When POLY has found an equilibrium, the equilibrium Gibbs energy surface is compared to the mesh to assure that no grid point is below the surface, i.e. a global minimization has been reached.

Global Minimization is now performed by default in single-point or stepping or mapping equilibrium calculations, but can of course be turned off (and on again by repeating the command-sequence of ADVANCED_OPTIONS GLOBAL_MINIMIZATION) by the user for specific purposes. This means that truly stable equilibrium should be guaranteed for single-points, stepping and mapping calculations.
 * A completely new stepping and mapping procedure that ensures Global Minimization everywhere it is critical has been developed and been made available in TCCS/TCW5. These newly re-written STEP/MAP routines are very important for stepping/mapping calculations in multicomponent systems where there are complex miscibility gaps in some phases, and

it does not require having any ¡°good¡± guess of starting points. Therefore, TCCS/TCW5 can automatically handle complex solution phases with single or multiple miscibility gaps [for instance, a solution phase that is thermodynamically described as a single phase in a Thermo-Calc database, such as FCC, BCC or HCP phases, may be split into two or several composition-sets/phases that are presented in an equilibrium state as metallic phase(s), carbide(s), nitride(s), carbonitride(s), nitrocarbide(s), and so on], and can thus ensure the correct and complete phase diagrams and property diagrams in multicomponent systems, without bothering staring points.

Together with the PARROT module, the POLY module is also used for critical assessment of experimental data in order to develop thermodynamic databases. The POLY module uses the Gibbs Energy System (GES) for modeling and data manipulations of the thermodynamic properties of each phase.

The following commands are available in the POLY module:

```
POLY_3:?
 ADD_INITIAL_EQUILIBRIUM  EXIT                     REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE              SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                     SELECT_EQUILIBRIUM
 BACK                     INFORMATION              SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE       SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS          SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM         SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA  SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS              SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS             SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN          SET_START_VALUE
 DELETE_SYMBOL            MAP                      SHOW_VALUE
 ENTER_SYMBOL             POST                     STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES          TABULATE
POLY_3:
```

Note that, since TCCS, the SPECIAL_OPTIONS and SET_MINIMIZAION_OPTIONS commands (the later one was introduced in the TCCR version) has been merged into the new ADVANCED_OPTIONS command; and the RECOVER_START_VALUES command has been removed, due to that is not relevant to the POLY module anymore.

Revision History of the POLY-Module User’s Guide:

```
 Mar 1991  First release
                   (Edited by Bo Jansson and Bo Sundman)
 Oct 1993  Second revised release (with version J)
                   (Edited by Bo Jansson and Bo Sundman)
 Oct 1996  Third revised release (with version L)
                   (Edited by Bo Sundman)
 Nov 1998  Fourth revised release (with version M)
                   (Edited by Bo Sundman)
 Jun 2000  Fifth revised and extended release
                   (Edited by Pingfang Shi)
 Nov 2002  Sixth revised and extended release
                   (Edited by Pingfang Shi)
 May 2006  Eighth revised and extended release
                   (Edited by Pingfang Shi)
 Apr 2008  Ninth revised and extended release
                   (Edited by Pingfang Shi)
```

```
WHICH SUBJECT:  ?
```

WHICH SUBJECT

Specify a subject (or its abbreviation as long as it is unique, e.g., SIN, SIT, SOL, SPE, STATE, STEP, SYM, SYS, SUB, etc.) on which information should be given, from the following subjects that are important to the use of the POLY module:

```
 PURPOSE                GETTING STARTED          USER INTERFACE
 HELP                   MACRO FACILITY           PRIVATE FILES
 BASIC THERMODYNAMICS   SYSTEM AND PHASES        CONSTITUENTS AND SPECIES
 SUBLATTICES            COMPONENTS               SITE AND MOLE FRACTIONS
 COMPOSITION AND CONSTITUTION                    CONCENTRATION
 STATE VARIABLES        INTENSIVE VARIABLES      EXTENSIVE VARIABLES
```

DERIVED VARIABLES	UNITS	BASIC UNITS
SYSTEM UNITS	COMPONENT UNITS	PHASE UNITS
PHASE-COMPONENT UNITS	PHASE-SPECIES UNITS	USER-SPECIFIED UNITS
SYMBOLS	REFERENCE STATES	METASTABLE EQUILIBRIUM
CONDITIONS	AXIS-VARIABLES	SPECIAL OPTIONS
CALCULATIONS TYPES	SINGLE EQUILIBRIUM	INITIAL EQUILIBRIUM
STEPPING	SOLIDIFICATION PATH	PARAEQUILIBRIUM AND T0
MAPPING	PLOTTING OF DIAGRAMS	GLOBAL MINIMIZATION
DIAGRAM TYPES	BINARY DIAGRAMS	TERNARY DIAGRAMS
QUASI-BINARY DIAGRAMS	HIGHER ORDER DIAGRAMS	PROPERTY DIAGRAMS
POTENTIAL DIAGRAMS	POURBAIX DIAGRAMS	AQUEOUS SOLUTIONS
ORDER-DISORDER	TROUBLE SHOOTING	FAQ

If you are using the ED_EXP module (the sub-module of the PARROT module), you can also get detailed information of the following subject keywords which are relevant to the EX_EXP module:

EDEXP	for Edit-Experiment Module (ED-EXP)
EDPOLY	for Performance of POLY Commands in the ED_EXP Module
EDSPECIAL	for Special Commands only available in the ED_EXP Module
EDPOP	for Other Commands in the Experimental Data (POP or DOP) Files

WHICH SUBJECT: **state**

STATE VARIABLES

Standard State Variables and Partial Derivatives

****

Classic Thermodynamics deals only with systems that are in equilibrium, i.e., in an EQUILIBRIUM STATE (either as full equilibrium, or partial or local equilibrium) which is stable against internal fluctuations in a number of variables, such as temperature and composition. These variables that have defined values or properties at the equilibrium state are called STATE VARIABLES. Other examples of state variables are pressure (P), and chemical potential (m). Thermodynamics provides a number of relations between these state variables that make it possible to calculate the value of any other variable at equilibrium.

A state variable can be of two types, extensive or intensive. The value of an extensive variable, e.g., volume, depends on the size of the system, whereas the value of an intensive variable, e.g., temperature, is independent of the size of the system. Each type of state variable has a complementary variable of the other type. The variable complementing the volume is pressure, while the variable complementing the composition of a component is its chemical potential.

It is worth mentioning here that the activity of a component can always be obtained from its chemical potential using a simple mathematical relationship. It is also possible to choose any convenient reference state for the activity or the chemical potential. One of the advantages with a thermodynamic databank on a computer is that, in most cases, such reference state changes can be handled internally without troubling the user.

If the work that can be exchanged with the surroundings is limited to pressure-volume work, the state of equilibrium of a system can be obtained by assigning values to exactly N+2 state variables where N is the number of components of the system.

Note that the Thermo-Calc software distinguishes between components of a system and constituent (i.e., species) of a phase in the system. Many state variables require one or the other. By default, the elements are defined as the system components, but this definition can be changed with the POLY command DEFINE_COMPONENT. For instance, if the elements are Ca, Si and O, the another set of components can be defined as CaO, SiO and O2; in a pure water system, the components are normally defined as H2O and H+. However, one can not change the number of components when using this command.

A state variable is a defined thermodynamic quantity either for the whole system, or for a component in the system, or a species in a specific substitutional phase, or a constituent (i.e., a species on a specific sublattice site) in a specific solution phase.

The POLY module operates on a thermodynamic system in a stable or meta-stable or partial/local equilibrium state that is described by state variables.

Examples of state variables are temperature, mole fraction, chemical potential and activity of a component (in the system or in a specific phase), enthalpy (of the system or a specific phase), etc. In the POLY module, a general notational method has been designed for the important set of standard state variables and their partial derivatives (or called as derived variables).

Common examples of state variables in a defined system are:

```
 T              for temperature (K)
 P              for pressure (Pa)
 N              for total system size (in moles)
 B              for total system site (in grams)
 N(H)           for overall mole number of the hydrogen component
 B(H2O)         for overall mass (grams) of the H2O component
 X(FE)          for overall mole fraction of the FE component
 W(AL2O3)       for overall mass fraction of the AL2O3 component
 Y(HCP,CR#1)   for site fraction of the Cr species
                          on the first sublattice site in the HCP phase
 X(LIQUID,FE)   for mole fraction of the Fe component in the LIQUID phase
 W(FCC,C)       for mass fraction of the C component in the FCC phase
 NP(BCC)        for mole number of the BCC phase
 BP(BCC)        for mass (grams) of the BCC phase
 VP(BCC)        for volume (m3) of the BCC phase
 DGM(BCC)       for driving force of the BCC phase per mole of components
 QF(SIGMA)     for phase stability function of the SIGMA phase
 MUR(C)         for chemical potential of the C component
                          (with regard to its reference state)
 ACR(C)         for activity of the C component
                          (with regard to its reference state)
 LNACR(C)       fatural logarithm of activity of the C component
                          [lnACR(C)=MUR(C)/RT]
 MUR(FE+3,AQ)  for chemical potential of the Fe+3 species
                          related to the aqueous solution phase
 ACR(FE+3,AQ)  for activity of the Fe+3 species
                          related to the aqueous solution phase
 LNACR(FE+3,AQ)        for natural logarithm of activity of the Fe+3 species
                          related to the aqueous solution phase
                          [lnACR(FE+3,AQ)=MUR(FE+3,AQ)/RT]
 HM             for total enthalpy per mole component in the system
 HM(FCC)        for enthalpy per mole component of the FCC phase
 HM.T           for heat capacity per mole of components
                          in the system (in J/mol/K)
 HM(FCC).T      for heat capacity per mole of components
                          of the FCC phase (in J/mol/K)
 P.T            for the slope delta_P/delta_T of a phase boundary
                          on a P-T phase diagram. Note that the equilibrium
                          with a phase assemblage must have been calculated.
 T.W(SI)        for the slope delta_T/delta_W(Si) of a phase boundary
                          on a T-W(Si) phase diagram with regard to
                          mass of the component in the system
 T.X(LIQ,CR)    for the slope delta_T/delta_X(Liq,Cr) of a phase boundary
                          on a T-X(Liq,Cr) phase diagram with regard to
                          mole fraction of the component in the phase

  Many more ‡     >>> see details below and in the document of
                                Thermo-Calc Software System
                                **************************
```

Note that the state variables involving components can be used for the defined components, but not for any species. To define new components in a defined system, the DEFINE_COMPONENT command should be used.

The basic intensive and extensive variables which are suitable in the POLY module of in the Thermo-Calc software system are listed and briefly described in Table 1 (of the document Thermo-Calc Software System), and are also be dealt with in the following subject-keywords when using the on-line help feature of the POLY module:

```
  INFO INTENSIVE VARIABLES    For Various Intensive State Variables
  INFO EXTENSIVE VARIABLES    For Various Extensive State Variables
```

Derivatives of state variables can be evaluated using a dot "." between two state variables. Many derived variables of a defined system, or of a certain system component, or of a given phase, or of a specific component in a defined phase, can be easily obtained using appropriate partial

```
 derivatives of state variables, such as heat capacity, thermal expansivity,
 isothermal compressibility, among others. For the details of various
 derived variables which are suitable in the POLY and POST modules of the
 Thermo-Calc software system, please refer to Section 2.6 in the document
 Thermo-Calc Software System, and also refer to the on-line help feature
 of the POLY module:
   INFO DERIVED VARIABLES      For Derived Variables (Partial Derivatives)

 Note that the lists of various state variables in the subject-keywords
 INTENSIVE VARIABLES and EXTENSIVE VARIABLES, as well as of derived variables
 (partial derivatives), are not exhaustive, but many other remaining state
 variables can be obtained through direct calls or by using combinations of
 the predefined state variables (such as those listed in the subject-keyword
 DERIVED VARIABLES (for various derived variables or partial derivatives)
 or user-specified ones. For more details, please refer to Sections 2.5
 [Equilibrium State and State Variables] and 2.6 [Derived Variables (Partial
 Derivatives)] in the document Thermo-Calc Software System.

WHICH SUBJECT:
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ We can list the current equilibrium by
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  ?
 OPTIONS

  The user may select the output units and formats by optionally specifying
  a combination of the following letters:
    Fraction order:   V means VALUE ORDER
                      A means ALPHABETICAL ORDER
    Fraction type:    W means MASS FRACTION
                      X means MOLE FRACTION
    Composition:      C means only COMPOSITION
                      N means CONSTITUTION and COMPOSITION.
    Phase:            S means including only STABLE PHASES
                      P means including ALL NON-SUSPENDED PHASES.

  Default is VWCS. If the output should be in mole fraction, then give
  VXCS or just X.

Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: PBIN

 Conditions:
 X(FE)=0.1234, P=1E5, N=1, T=1319.08
 DEGREES OF FREEDOM 0

 Temperature   1319.08 K (  1045.93 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.74204E+01
 Total Gibbs energy -2.71048E+04,  Enthalpy  2.18963E+04,  Volume  8.37682E-07

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       8.7660E-01  6.0440E-01 1.0000E+00  6.8849E-13 GRAPHITE
 FE                      1.2340E-01  3.9560E-01 8.9831E-01 -1.1762E+03 BCC_A2

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 8.6693E-01, Mass 1.0413E+01, Volume fraction 0.0000E+00  Mass fractions:
 C   1.00000E+00  FE  0.00000E+00

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.3307E-01, Mass 7.0077E+00, Volume fraction 1.0000E+00  Mass fractions:
 FE  9.83420E-01  C   1.65804E-02
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The actual conditions are listed by the list-equil command but
POLY_3: @@ can be obtained also by
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 X(FE)=0.1234, P=1E5, N=1, T=1319.08
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The meaning of the state variables T, P, X, N  and many others
POLY_3: @@ are explained by the INFO command
```

POLY_3: **INFO**
... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/: **state**
STATE VARIABLES

Standard State Variables and Partial Derivatives
****

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X(FE)	for overall mole fraction of the FE component
W(AL2O3)	for overall mass fraction of the AL2O3 component
Y(HCP,CR#1)	for site fraction of the Cr species on the first sublattice site in the HCP phase
X(LIQUID,FE)	for mole fraction of the Fe component in the LIQUID phase
W(FCC,C)	for mass fraction of the C component in the FCC phase

```
 NP(BCC)        for mole number of the BCC phase
 BP(BCC)        for mass (grams) of the BCC phase
 VP(BCC)        for volume (m3) of the BCC phase
 DGM(BCC)       for driving force of the BCC phase per mole of components
 QF(SIGMA)     for phase stability function of the SIGMA phase
 MUR(C)         for chemical potential of the C component
                          (with regard to its reference state)
 ACR(C)         for activity of the C component
                          (with regard to its reference state)
 LNACR(C)       fatural logarithm of activity of the C component
                          [lnACR(C)=MUR(C)/RT]
 MUR(FE+3,AQ)  for chemical potential of the Fe+3 species
                          related to the aqueous solution phase
 ACR(FE+3,AQ)  for activity of the Fe+3 species
                          related to the aqueous solution phase
 LNACR(FE+3,AQ)        for natural logarithm of activity of the Fe+3 species
                          related to the aqueous solution phase
                          [lnACR(FE+3,AQ)=MUR(FE+3,AQ)/RT]
 HM             for total enthalpy per mole component in the system
 HM(FCC)        for enthalpy per mole component of the FCC phase
 HM.T           for heat capacity per mole of components
                          in the system (in J/mol/K)
 HM(FCC).T      for heat capacity per mole of components
                          of the FCC phase (in J/mol/K)
 P.T            for the slope delta_P/delta_T of a phase boundary
                          on a P-T phase diagram. Note that the equilibrium
                          with a phase assemblage must have been calculated.
 T.W(SI)        for the slope delta_T/delta_W(Si) of a phase boundary
                          on a T-W(Si) phase diagram with regard to
                          mass of the component in the system
 T.X(LIQ,CR)    for the slope delta_T/delta_X(Liq,Cr) of a phase boundary
                          on a T-X(Liq,Cr) phase diagram with regard to
                          mole fraction of the component in the phase

  Many more ‡     >>> see details below and in the document of
                                Thermo-Calc Software System
                                **************************
```

Note that the state variables involving components can be used for the defined components, but not for any species. To define new components in a defined system, the DEFINE_COMPONENT command should be used.

The basic intensive and extensive variables which are suitable in the POLY module of in the Thermo-Calc software system are listed and briefly described in Table 1 (of the document Thermo-Calc Software System), and are also be dealt with in the following subject-keywords when using the on-line help feature of the POLY module:

```
  INFO INTENSIVE VARIABLES    For Various Intensive State Variables
  INFO EXTENSIVE VARIABLES    For Various Extensive State Variables
```

Derivatives of state variables can be evaluated using a dot "." between two state variables. Many derived variables of a defined system, or of a certain system component, or of a given phase, or of a specific component in a defined phase, can be easily obtained using appropriate partial derivatives of state variables, such as heat capacity, thermal expansivity, isothermal compressibility, among others. For the details of various derived variables which are suitable in the POLY and POST modules of the Thermo-Calc software system, please refer to Section 2.6 in the document Thermo-Calc Software System, and also refer to the on-line help feature of the POLY module:

```
  INFO DERIVED VARIABLES      For Derived Variables (Partial Derivatives)
```

Note that the lists of various state variables in the subject-keywords INTENSIVE VARIABLES and EXTENSIVE VARIABLES, as well as of derived variables (partial derivatives), are not exhaustive, but many other remaining state variables can be obtained through direct calls or by using combinations of the predefined state variables (such as those listed in the subject-keyword DERIVED VARIABLES (for various derived variables or partial derivatives) or user-specified ones. For more details, please refer to Sections 2.5 [Equilibrium State and State Variables] and 2.6 [Derived Variables (Partial Derivatives)] in the document Thermo-Calc Software System.

```
WHICH SUBJECT:
POLY_3: @?<Hit_return_to_continue>
```

```
POLY_3: @@ The use of state variables as conditions is the key to the
POLY_3: @@ flexibility of TC. Each condition is set independently and
POLY_3: @@ any condition can be set as axis variable.
POLY_3: @@
POLY_3: @@ Now we just want to take away the graphite in order to calculate the
POLY_3: @@ metastable Fe-C diagram with cementite. We can list all phases by the
POLY_3: @@ LIST_STATUS command
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT              STATUS    REF. STATE     T(K)           P(Pa)
 VA                     ENTERED   SER
 C                      ENTERED   GRAPHITE       *              100000
 FE                     ENTERED   BCC_A2         *              100000
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 GRAPHITE               ENTERED    0.00000000E+00  8.66926312E-01
 FCC_A1                 ENTERED    0.00000000E+00  1.33073687E-01
 CEMENTITE              ENTERED   -5.29904061E-03  0.00000000E+00
 LIQUID                 ENTERED   -7.85895553E-02  0.00000000E+00
 BCC_A2                 ENTERED   -9.00754120E-02  0.00000000E+00
 HCP_A3                 ENTERED   -3.85804515E-01  0.00000000E+00
 CUB_A13                ENTERED   -4.71169903E-01  0.00000000E+00
 CBCC_A12               ENTERED   -5.62228159E-01  0.00000000E+00
 DIAMOND_FCC_A4         ENTERED   -6.79780053E-01  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 C    ENTERED    FE   ENTERED    FE+2 ENTERED    FE+3 ENTERED    VA   ENTERED
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The status is changed by the CHANGE_STATUS command
POLY_3: ch-st
   ... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): ?
 Phase name(s)

  In case of "phase" as the keyword, the names of the phases that shall
  have their status changes must be given (all on one line). A comma or
  space must be used as separator. The status to be assigned to the phases
  can also be given on the same line if preceded with an equal sign "=".
  Note that an asterisk, "*", can be used to denote all phases. The special
  notations "*S", i.e., a * directly followed by an S, means all suspended
  phases. In the same way, "*D" means all dormant phases, and "*E" means
  all entered phases.

Phase name(s): gra
Status: /ENTERED/:  sus
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT              STATUS    REF. STATE     T(K)           P(Pa)
 VA                     ENTERED   SER
 C                      ENTERED   GRAPHITE       *              100000
 FE                     ENTERED   BCC_A2         *              100000
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 FCC_A1                 ENTERED    0.00000000E+00  1.33073687E-01
 CEMENTITE              ENTERED   -5.29904061E-03  0.00000000E+00
 LIQUID                 ENTERED   -7.85895553E-02  0.00000000E+00
 BCC_A2                 ENTERED   -9.00754120E-02  0.00000000E+00
 HCP_A3                 ENTERED   -3.85804515E-01  0.00000000E+00
 CUB_A13                ENTERED   -4.71169903E-01  0.00000000E+00
 CBCC_A12               ENTERED   -5.62228159E-01  0.00000000E+00
 DIAMOND_FCC_A4         ENTERED   -6.79780053E-01  0.00000000E+00
 SUSPENDED PHASES:
 GRAPHITE
 *** STATUS FOR ALL SPECIES
 C    ENTERED    FE   ENTERED    FE+2 ENTERED    FE+3 ENTERED    VA   ENTERED
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Note that the graphite is listed as suspended this time.
POLY_3: @@ we try to calculate the equilibrium without graphite.
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
```

```
 Using global minimization procedure
 Calculated          824  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ A number of ,,, after a command means to accept default values.
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PBIN

 Conditions:
 X(FE)=0.1234, P=1E5, N=1, T=1319.08
 DEGREES OF FREEDOM 0

 Temperature   1319.08 K (  1045.93 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.74204E+01
 Total Gibbs energy -2.08664E+04,  Enthalpy  2.29690E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       8.7660E-01  6.0440E-01 1.9734E+00  7.4555E+03 GRAPHITE
 FE                      1.2340E-01  3.9560E-01 7.2125E-01 -3.5839E+03 BCC_A2

 DIAMOND_FCC_A4              Status ENTERED     Driving force  0.0000E+00
 Moles 8.3547E-01, Mass 1.0035E+01, Volume fraction 0.0000E+00  Mass fractions:
 C   1.00000E+00  FE  0.00000E+00

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.6453E-01, Mass 7.3856E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.33106E-01  C   6.68943E-02
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ It may seem surprising that diamond is stable but the total mole fraction
POLY_3: @@ of iron is less than 0.5, so we are on the carbon rich side
POLY_3: @@ of cementite, and it is reasonable.
POLY_3:
POLY_3: @@ Now try to map the metastable diagram now
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
```

```
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
 Generating start point  31
 Generating start point  32

 Phase region boundary   1 at:   5.000E-01  3.100E+02
     BCC_A2
  ** DIAMOND_FCC_A4
 Calculated..             2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   5.000E-01  3.000E+02
     BCC_A2
  ** DIAMOND_FCC_A4
 Calculated.           24  equilibria

 Phase region boundary   3 at:   4.999E-01  8.605E+02
     BCC_A2
  ** CEMENTITE
  ** DIAMOND_FCC_A4

 Phase region boundary   4 at:   8.749E-01  8.605E+02
     BCC_A2
  ** CEMENTITE
 Calculated.            7  equilibria

       :
       :
       :

 Phase region boundary  44 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_FCC_A4
 Calculated.           42  equilibria
 Terminating at known equilibrium

 Phase region boundary  45 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_FCC_A4
 Calculated..            2  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

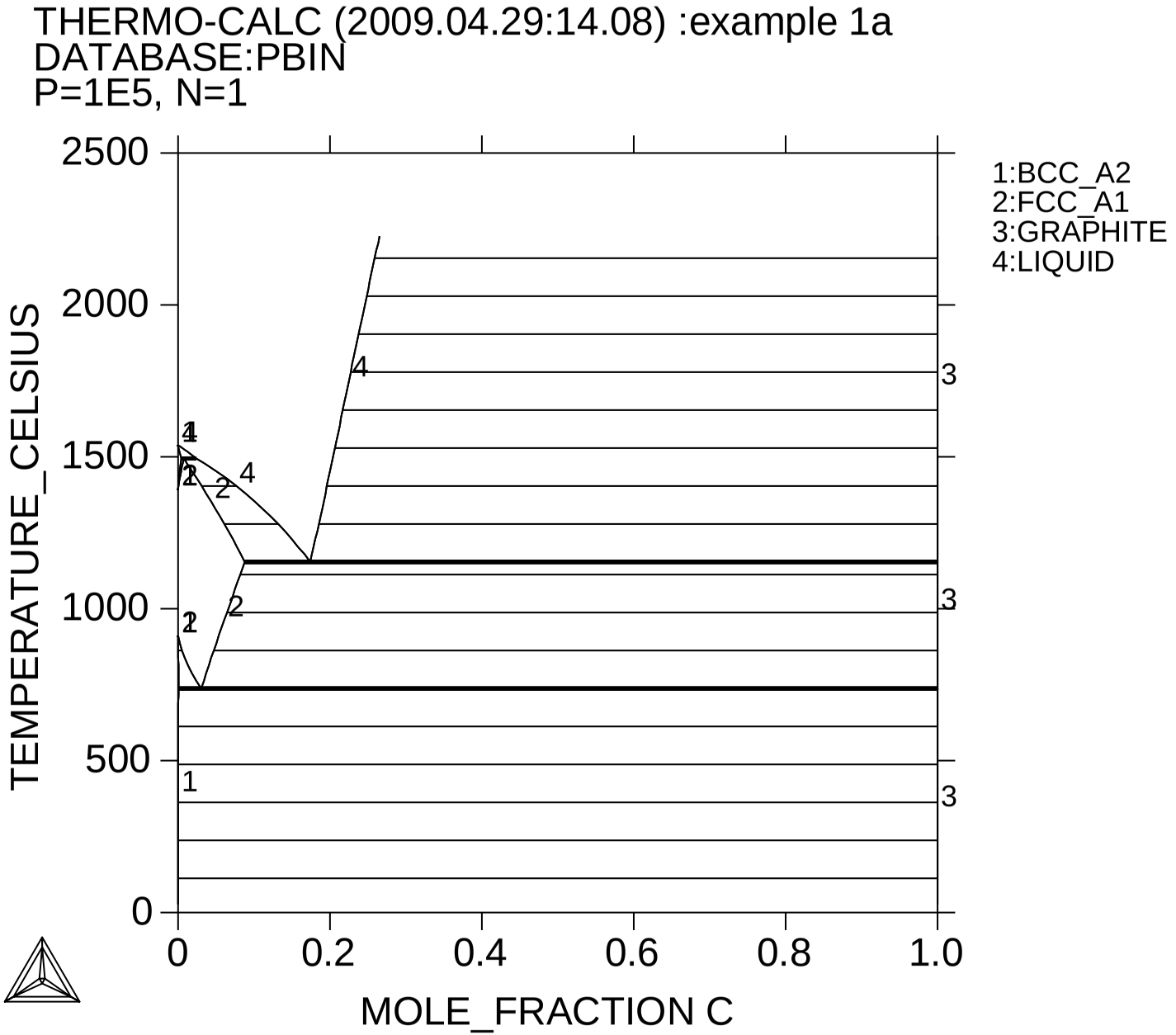
 Phase region boundary  46 at:   9.941E-01  1.794E+03
     LIQUID
  ** BCC_A2
 Calculated.            2  equilibria
 Terminating at known equilibrium

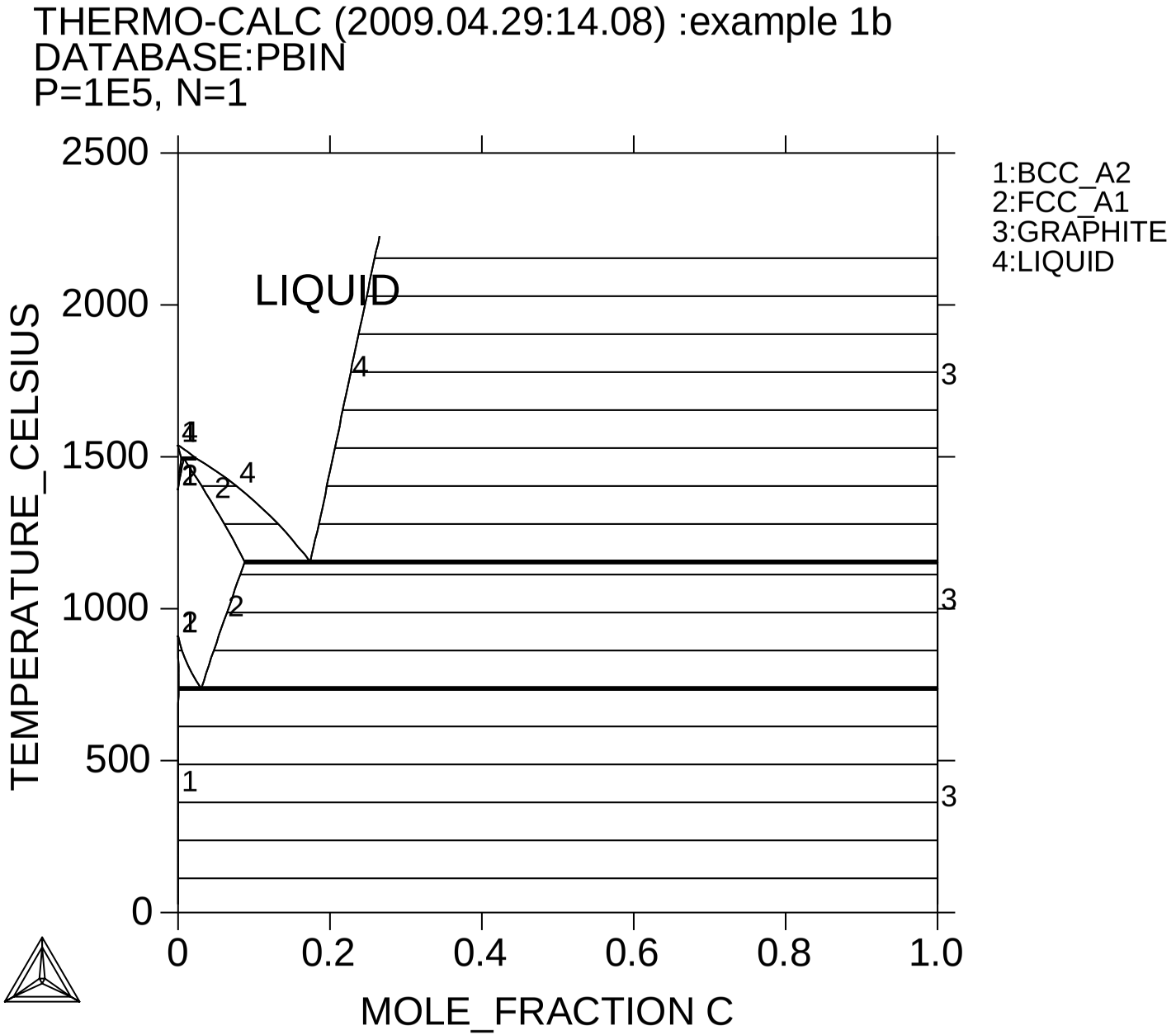
 Phase region boundary  47 at:   9.941E-01  1.794E+03
     LIQUID
  ** BCC_A2
 Calculated           12  equilibria
 *** BUFFER SAVED ON FILE: BINARY.POLY3
 CPU time for mapping           2  seconds
POLY_3:
POLY_3: post
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x m-f C
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-tieline
   ... the command in full is SET_TIELINE_STATUS
PLOTTING EVERY TIE-LINE NO /5/:  5
```

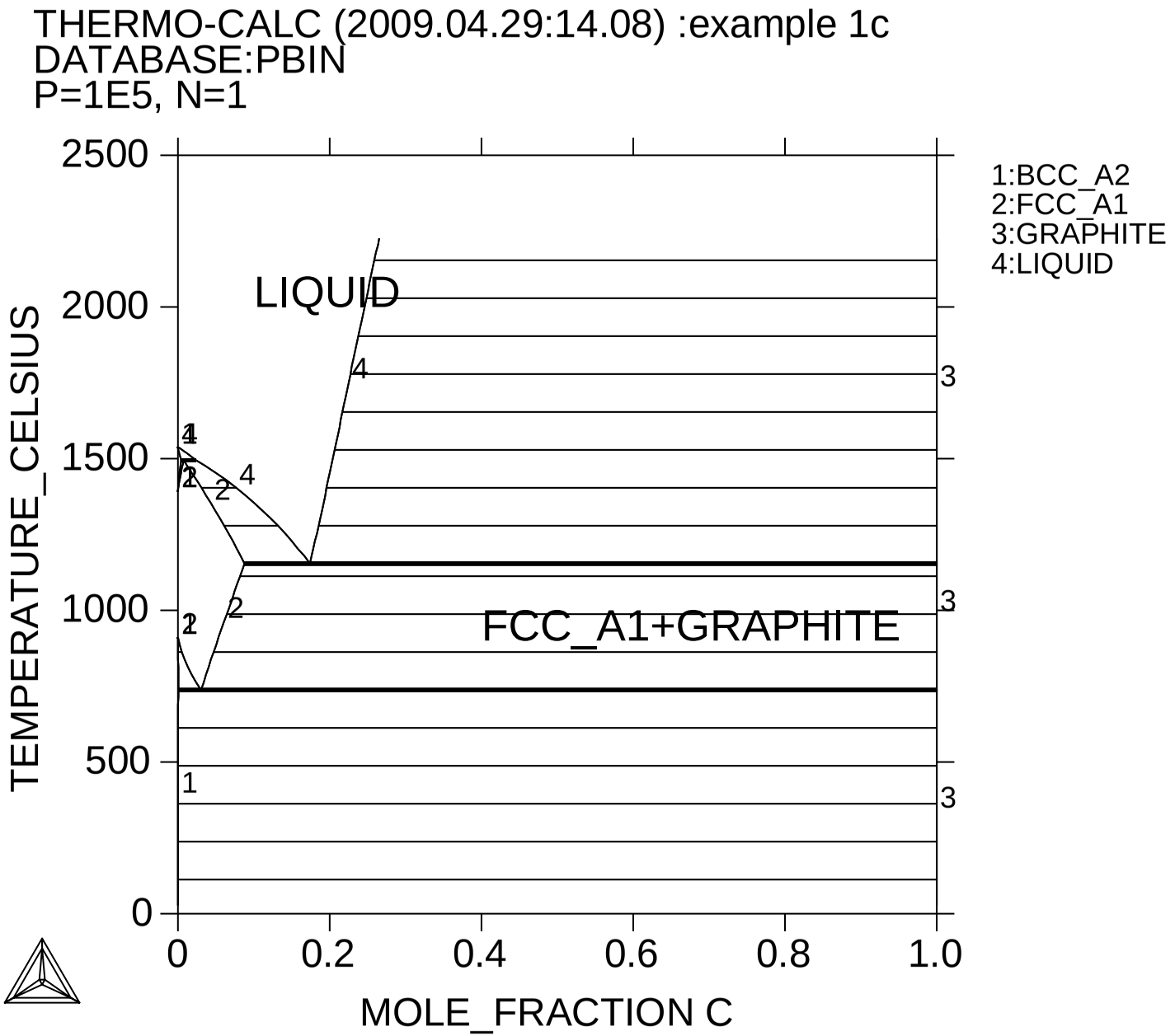
POST: **s-p-f ##1,,,,,,**
POST:
POST: **set-title example 1f**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ The previous stable diagram is also plotted. The reason is that***
POST: ***@@ we never removed it from the workspace (It can be done with a SAVE***
POST: ***@@ command, please read about this command).***
POST: ***@@***
POST: ***@@ It may be surprising to find that diamond is more stable than***
POST: ***@@ cementite at low temperature. However, one would never find***
POST: ***@@ diamonds in steel, unfortunately, as graphite would form first.***
POST: ***@@***
POST: ***@@ Now change the axis to composition, use weight-percent of carbon***
POST: **s-d-a x**
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : **?**
UNKNOWN QUESTION VARIABLE :
VARIABLE : **w-p**
FOR COMPONENT : **c**
POST: **set-title example 1g**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ The tie-lines now obscure the diagram, take them away***
POST: ***@@ Also change the scale of the x and y axis***
POST: **s-t-s 0**
... the command in full is SET_TIELINE_STATUS
POST: **s-s x n 0 5**
... the command in full is SET_SCALING_STATUS
POST: **s-s y n 600 1600**
... the command in full is SET_SCALING_STATUS
POST: **set-title example 1h**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ Finally add some nice labels***
POST: **set-lab n**
... the command in full is SET_LABEL_CURVE_OPTION
POST: **add 2 1250**
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 824 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
Stable phases are: CEMENTIT+FCC_A1
Text size: /.3999999762/:
POST: **set-title example 1i**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **add 1.5 900**
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 824 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s

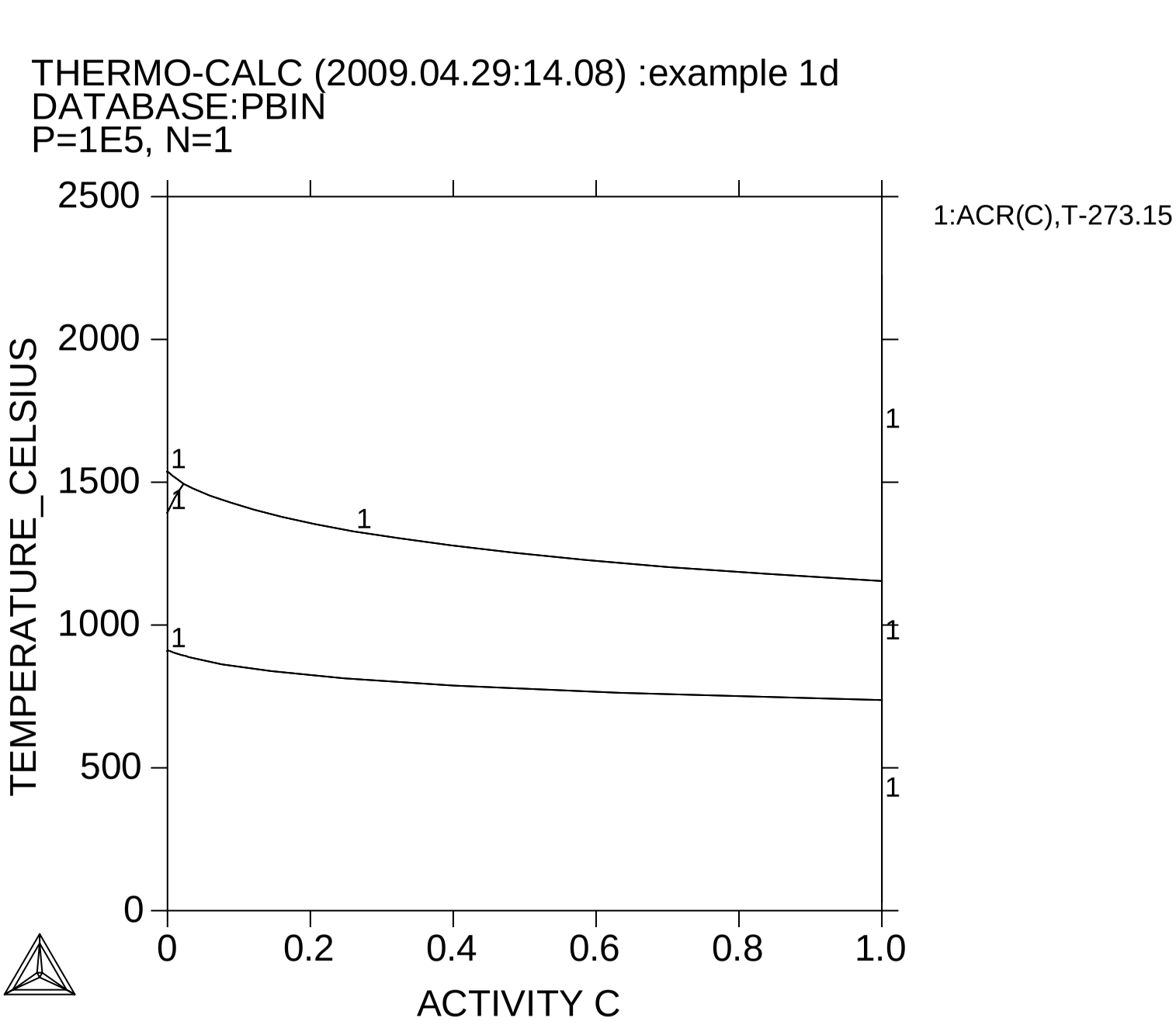
```
 Stable phases are: BCC_A2+CEMENTIT
Text size: /.3999999762/:
POST: add 1.5 700
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated          824  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_A2+DIAMOND_
Text size: /.3999999762/:
POST: add .2 1500
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated          824  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: FCC_A1
Text size: /.3999999762/:
POST: set-title example 1j
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ As graphite is suspended cementite is the stable carbide
POST: @@ so that is the phase that will be listed in the two-phase regions.
POST: @@ The label for the FCC region is a bit too high, move it down
POST: modify
   ... the command in full is MODIFY_LABEL_TEXT
 These labels are defined
 No   1 at  2.00000E+00 1.25000E+03 : CEMENTIT+FCC_A1
 No   2 at  1.50000E+00 9.00000E+02 : BCC_A2+CEMENTIT
 No   3 at  1.50000E+00 7.00000E+02 : BCC_A2+DIAMOND_
 No   4 at  2.00000E-01 1.50000E+03 : FCC_A1

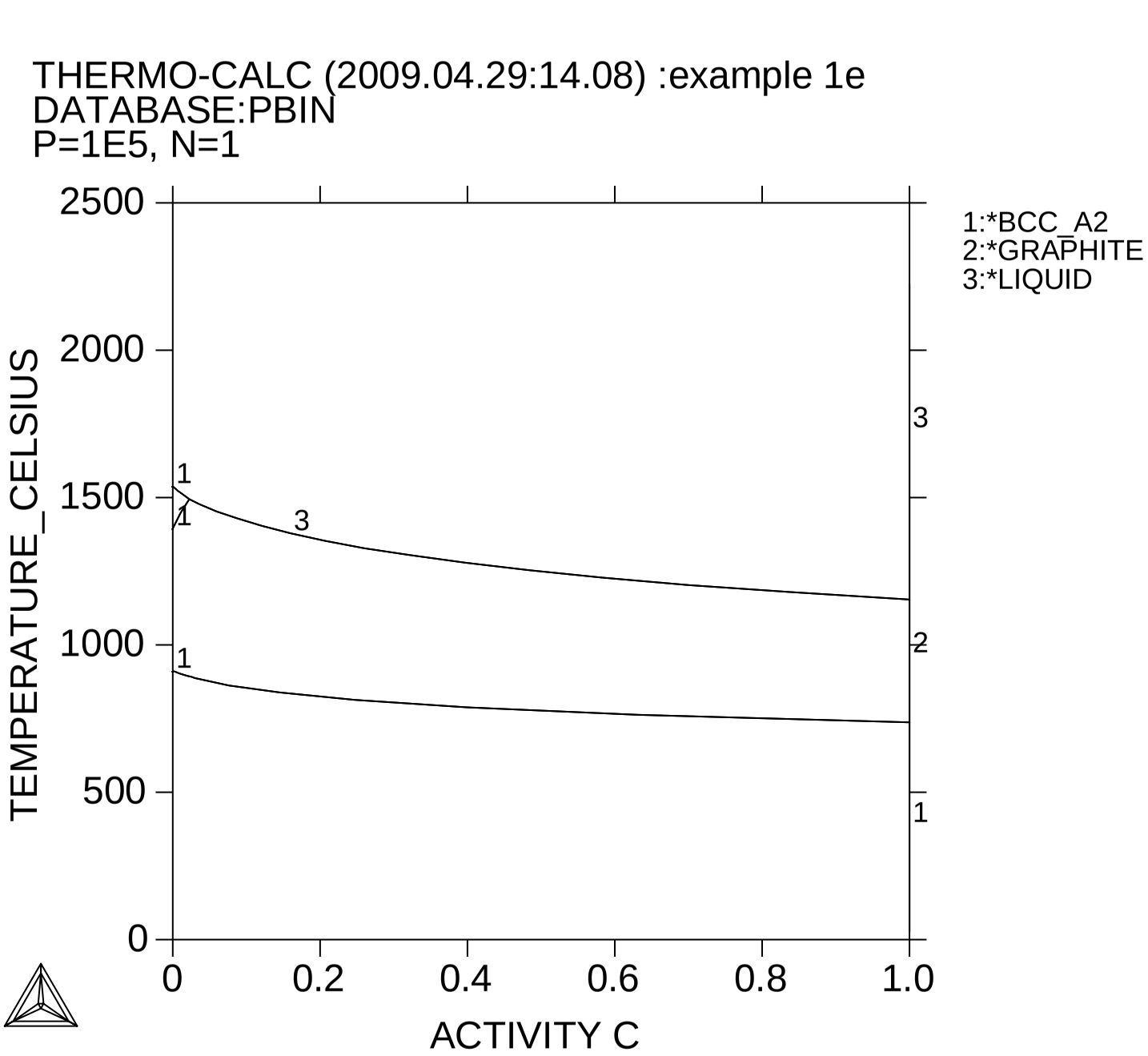
Which label to modify? /4/:
New X coordinate /.2/:  .2
New Y coordinate /1500/:  1300
New text /FCC_A1/:
POST: set-title example 1k
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
 CPU time            4  seconds
```


THERMO-CALC (2009.04.29:14.08) :example 1a
DATABASE:PBIN
P=1E5, N=1
2500
2000
1500
1000
500
0
TEMPERATURE_CELSIUS
0
0.2
0.4
0.6
0.8
1.0
MOLE_FRACTION C
1:BCC_A2
2:FCC_A1
3:GRAPHITE
4:LIQUID

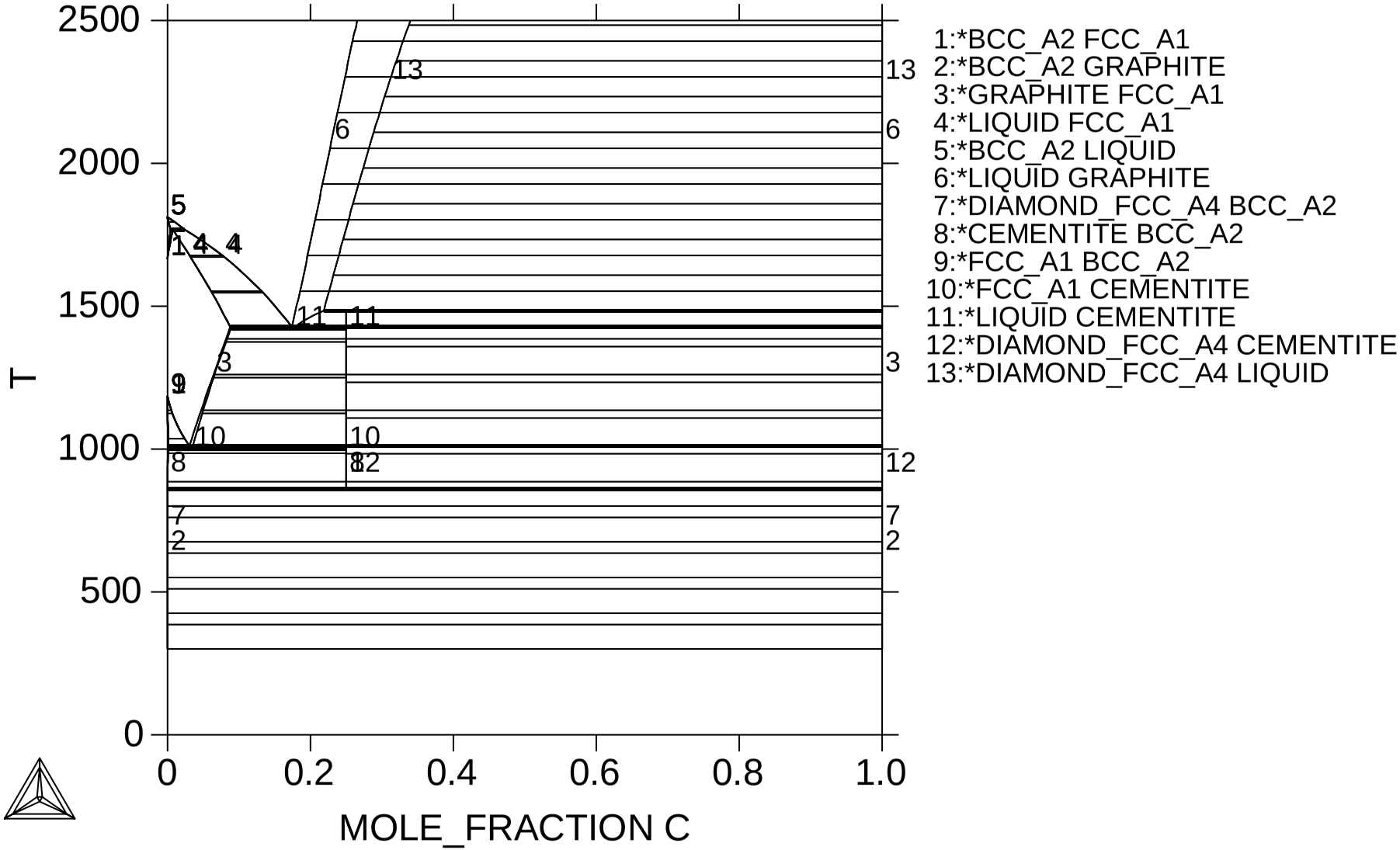

THERMO-CALC (2009.04.29:14.08) :example 1b
DATABASE:PBIN
P=1E5, N=1
2500
2000
1500
1000
500
0
TEMPERATURE_CELSIUS
0
0.2
0.4
0.6
0.8
1.0
MOLE_FRACTION C
LIQUID
1:BCC_A2
2:FCC_A1
3:GRAPHITE
4:LIQUID


THERMO-CALC (2009.04.29:14.08) :example 1c
DATABASE:PBIN
P=1E5, N=1
2500
2000
1500
1000
500
0
TEMPERATURE_CELSIUS
0
0.2
0.4
0.6
0.8
1.0
MOLE_FRACTION C
LIQUID
FCC_A1+GRAPHITE
1:BCC_A2
2:FCC_A1
3:GRAPHITE
4:LIQUID

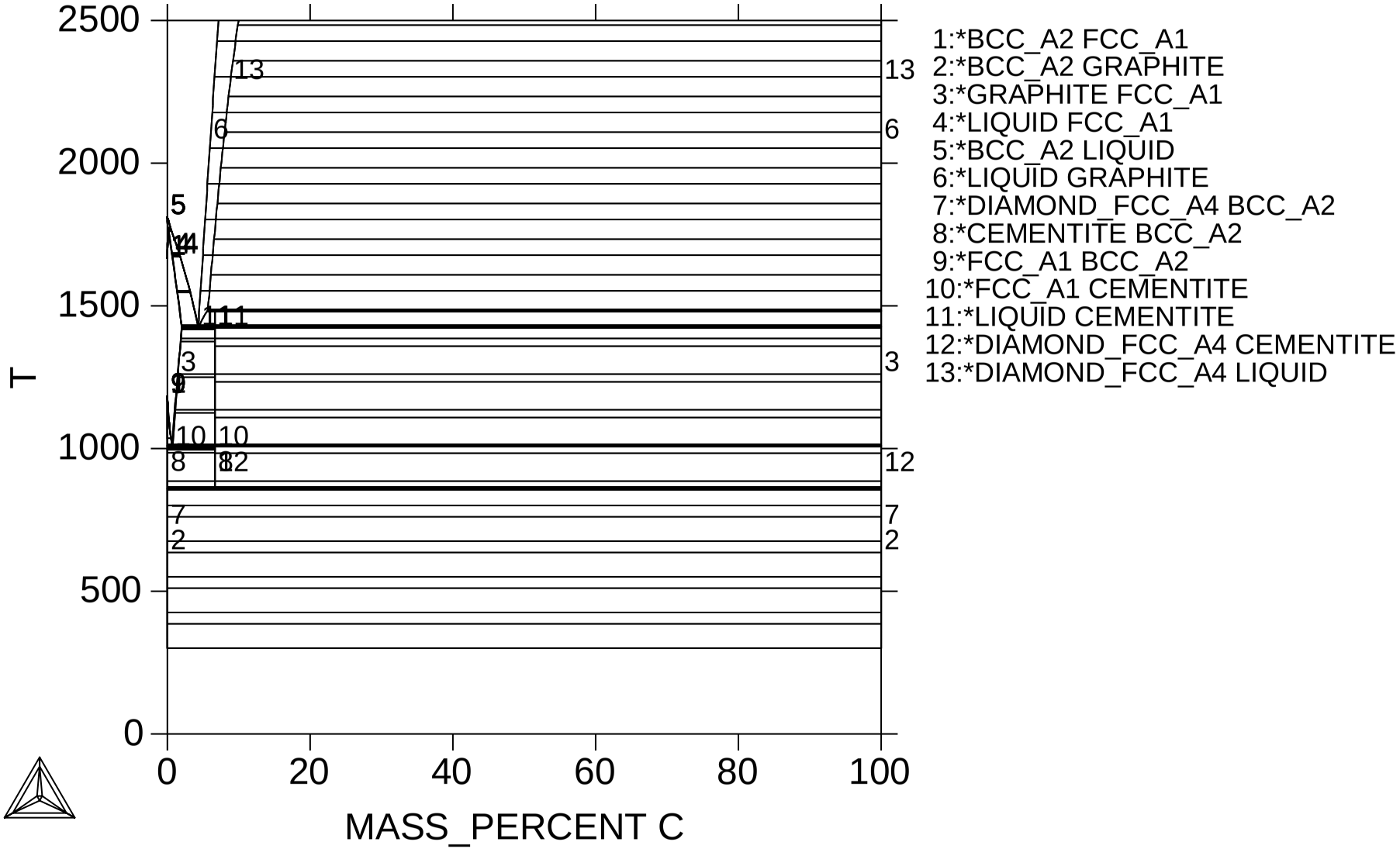

THERMO-CALC (2009.04.29:14.08) :example 1d
DATABASE:PBIN
P=1E5, N=1
2500
2000
1500
1000
500
0
TEMPERATURE_CELSIUS
0
0.2
0.4
0.6
0.8
1.0
ACTIVITY C
1:ACR(C),T-273.15


THERMO-CALC (2009.04.29:14.08) :example 1e
DATABASE:PBIN
P=1E5, N=1
2500
2000
1500
1000
500
0
TEMPERATURE_CELSIUS
0
0.2
0.4
0.6
0.8
1.0
ACTIVITY C
1:*BCC_A2
2:*GRAPHITE
3:*LIQUID
1
1
3
1
3
2
1

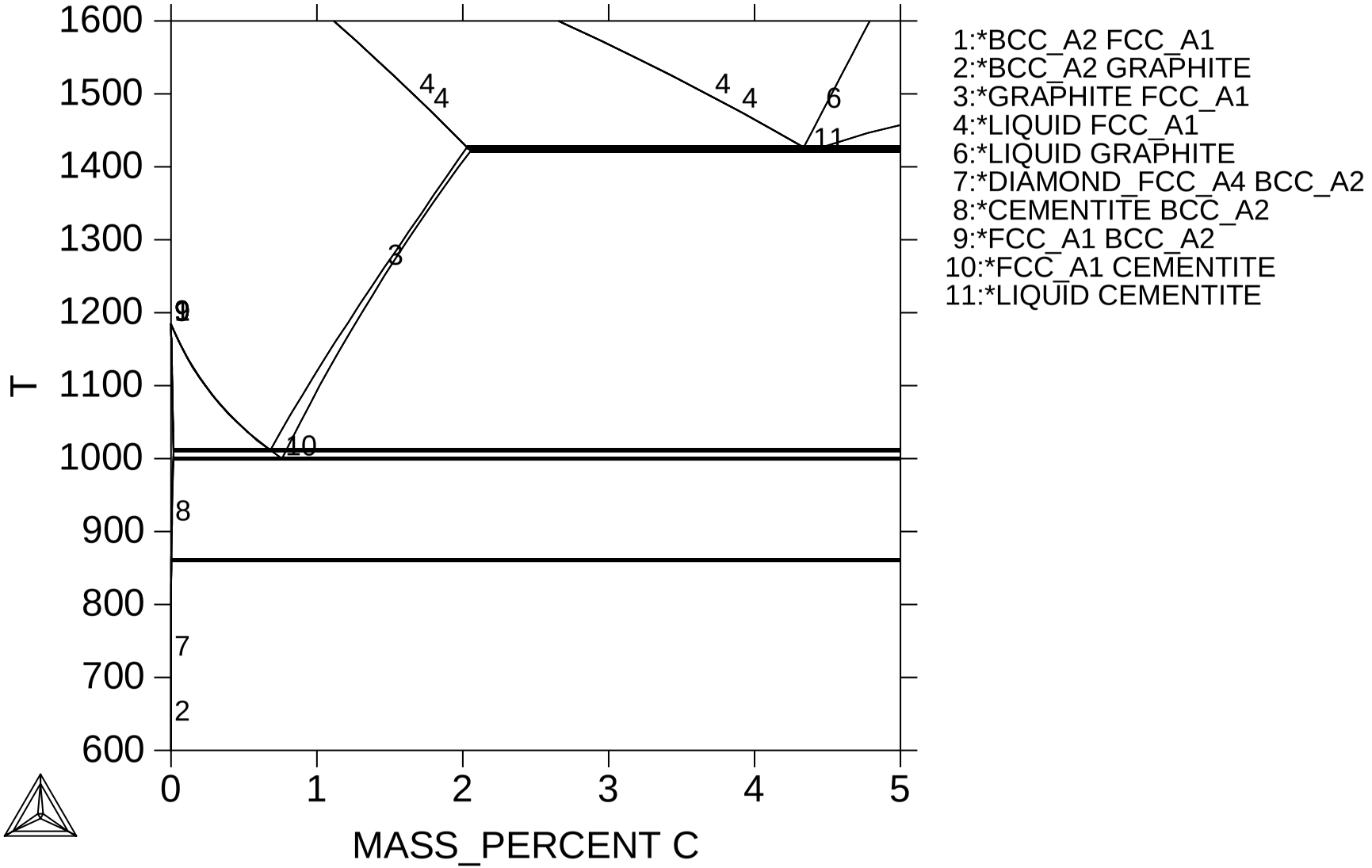
THERMO-CALC (2009.04.29:14.08) :example 1f
DATABASE:PBIN
P=1E5, N=1

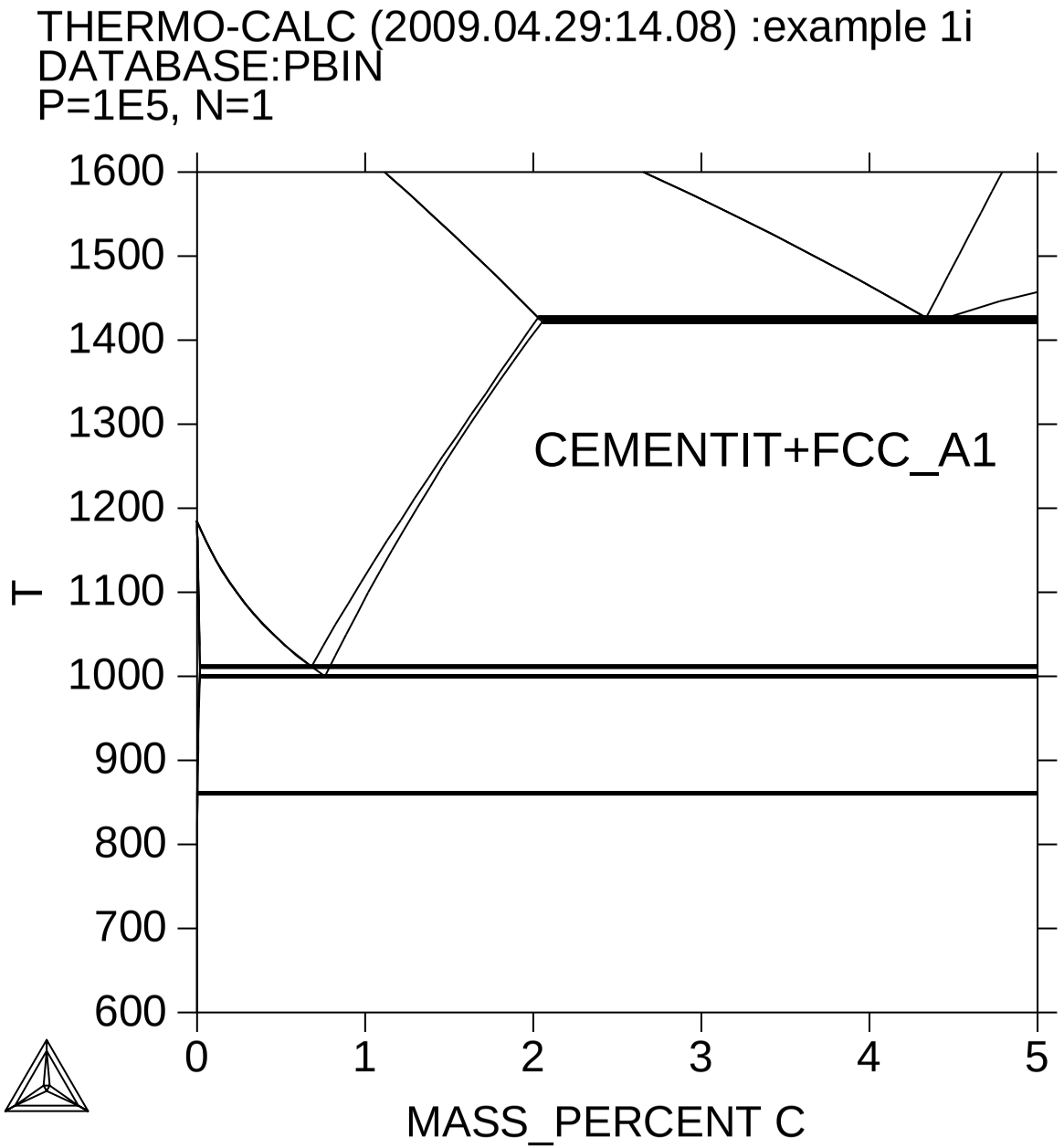


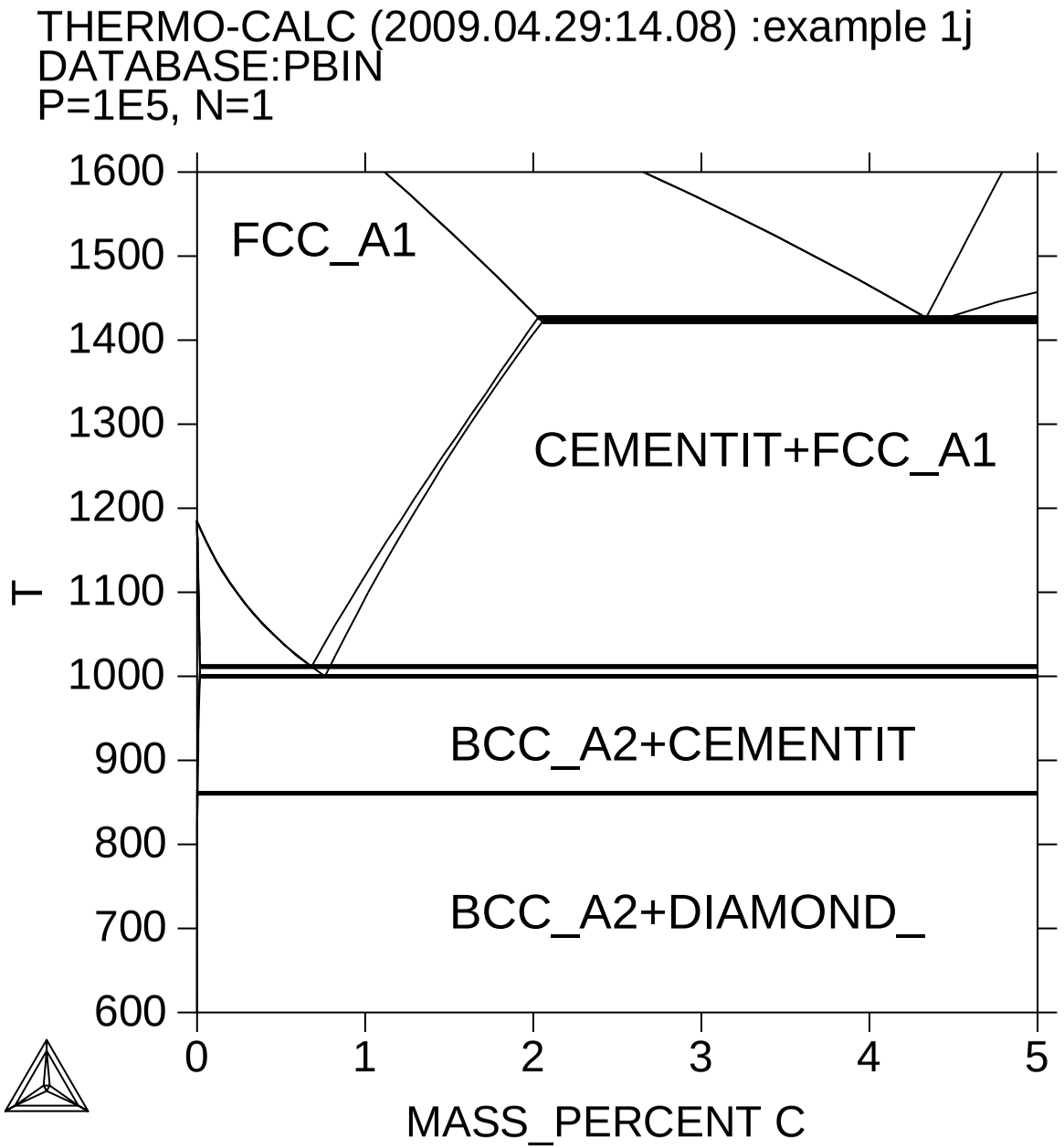
THERMO-CALC (2009.04.29:14.08) :example 1g
DATABASE:PBIN
P=1E5, N=1

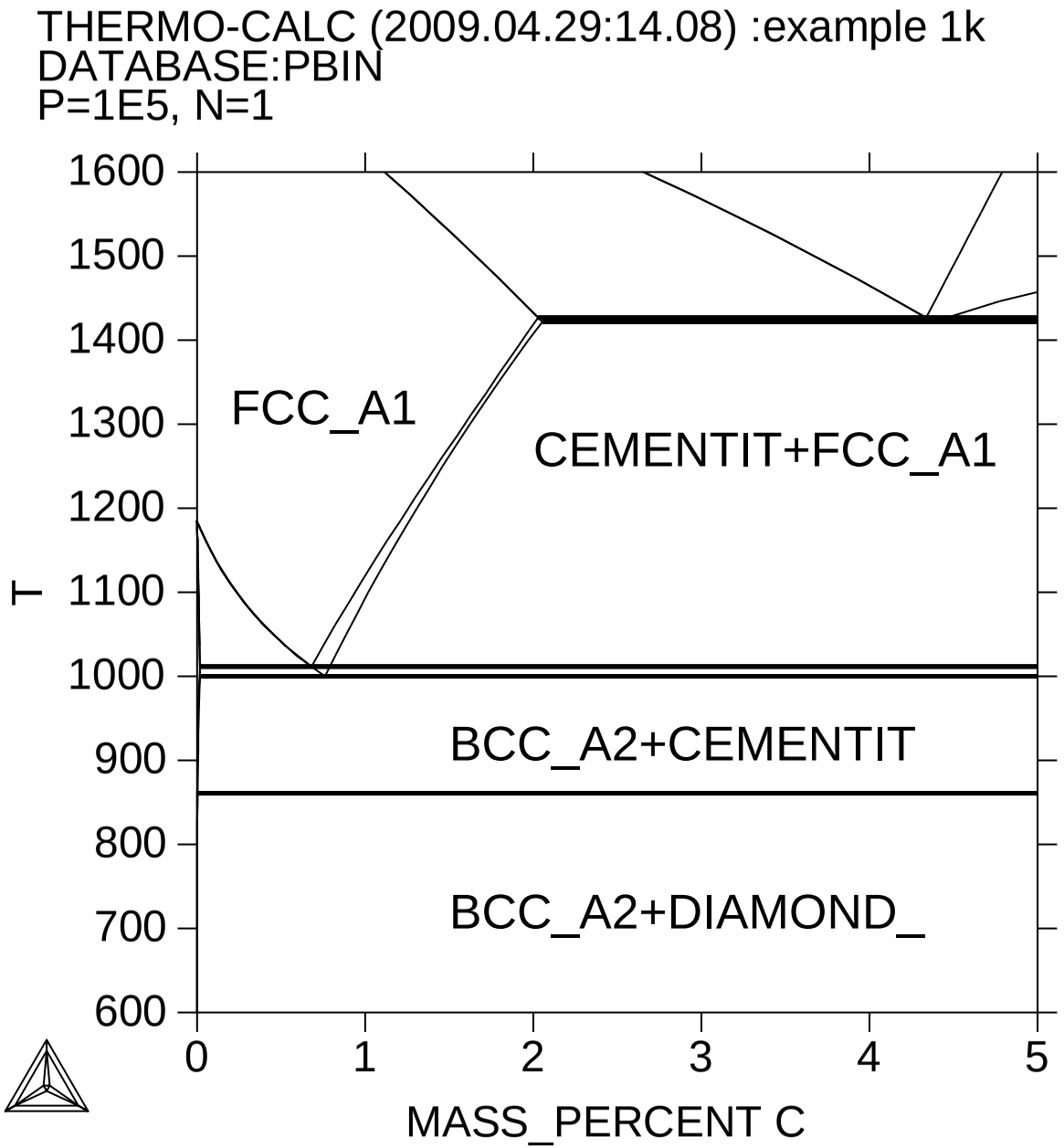


THERMO-CALC (2009.04.29:14.08) :example 1h
DATABASE:PBIN
P=1E5, N=1




THERMO-CALC (2009.04.29:14.08) :example 1i
DATABASE:PBIN
P=1E5, N=1
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
T
CEMENTIT+FCC_A1
0
1
2
3
4
5
MASS_PERCENT C


THERMO-CALC (2009.04.29:14.08) :example 1j
DATABASE:PBIN
P=1E5, N=1
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
T
FCC_A1
CEMENTIT+FCC_A1
BCC_A2+CEMENTIT
BCC_A2+DIAMOND_
0
1
2
3
4
5
MASS_PERCENT C


THERMO-CALC (2009.04.29:14.08) :example 1k
DATABASE:PBIN
P=1E5, N=1
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
T
FCC_A1
CEMENTIT+FCC_A1
BCC_A2+CEMENTIT
BCC_A2+DIAMOND_
0
1
2
3
4
5
MASS_PERCENT C

2

Plotting of thermodynamic functions in unary, binary and ternary systems and working with partial derivatives and partial quantities

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Thermodynamic properties
SYS: @@
SYS: set-log ex02,,
SYS:
SYS:
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw ssol2
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Alloy Solutions Database v2

 VA  DEFINED
 B2_BCC                  L12_FCC                 AL5FE4:
   REJECTED
 GAS:G                   AQUEOUS:A               WATER:A
   REJECTED
TDB_SSOL2: @@ Pure Fe is selected as unary system
TDB_SSOL2: d-sys fe
   ... the command in full is DEFINE_SYSTEM
 FE  DEFINED
TDB_SSOL2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
   'H. Du and M. Hillert, revision; C-Fe-N'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
       September 1989'
 -OK-
TDB_SSOL2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ In POLY-3 we first define a single equilibrium
POLY_3: s-c t=300,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated            7  grid points in            0  s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL2

 Conditions:
 T=300, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    300.00 K (    26.85 C),  Pressure  1.000000E+05
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```
 Number of moles of components  1.00000E+00,  Mass in grams  5.58470E+01
 Total Gibbs energy -8.18336E+03,  Enthalpy  4.66785E+01,  Volume  7.10115E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 FE                      1.0000E+00  1.0000E+00 3.7600E-02 -8.1834E+03 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.5847E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  1.00000E+00
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ We set T as axis variable
POLY_3: s-a-v
   ... the command in full is SET_AXIS_VARIABLE
Axis number: /1/:  1
Condition /NONE/:  t
Min value /0/:  300
Max value /1/:  2000
Increment /42.5/:  42.5
POLY_3: @@ We always save in order to be able to come back to this point
POLY_3: save tcex02a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ Step along the axis
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  NORMAL
 No initial equilibrium, using default
 Step will start from axis value    300.000
 Global calculation of initial equilibrium ....OK

 Phase Region from    300.000     for:
     BCC_A2
 Global test at  3.80000E+02 .... OK
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
 Global check of adding phase at  1.18481E+03
 Calculated    91 equilibria

 Phase Region from    1184.81     for:
     BCC_A2
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    1184.81     for:
     FCC_A1
 Global test at  1.26000E+03 .... OK
 Global test at  1.36000E+03 .... OK
 Global test at  1.46000E+03 .... OK
 Global test at  1.56000E+03 .... OK
 Global test at  1.66000E+03 .... OK
 Global check of adding phase at  1.66748E+03
 Calculated    51 equilibria

 Phase Region from    1667.48     for:
     BCC_A2
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    1667.48     for:
     BCC_A2
 Global test at  1.74000E+03 .... OK
 Global check of adding phase at  1.81096E+03
 Calculated    18 equilibria

 Phase Region from    1810.96     for:
     LIQUID
     BCC_A2
 Calculated     2 equilibria
```

```
 Phase Region from    1810.96     for:
     LIQUID
 Global test at  1.89000E+03 .... OK
 Global test at  1.99000E+03 .... OK
 Terminating at    2000.00
 Calculated    22 equilibria
 *** Buffer saved on file: tcex02a.POLY3
POLY_3: @@ Post processing is the essential part of this example
POLY_3: @@ We will plot Gm, Hm and Cp for some phases
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,
POST:
POST:
POST: @@ The  x-axis will be the temperature in Kelvin
POST: s-d-a x
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
 UNKNOWN QUESTION VARIABLE :
VARIABLE : t-k
POST: @@ The phases for which Gm shall be plotted must be defined
POST: @@ in a table
POST: ent tab
   ... the command in full is ENTER_SYMBOL
Name: g1
Variable(s): gm(bcc) gm(fcc) gm(liq) gm(hcp)
&
POST:
POST: @@ The table is set as y-axis and all columns included
POST: s-d-a y g1
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: set-title example 2a
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@
POST: @@ The magnitude makes it difficult to see anything. Enter
POST: @@ functions for the differences with respect to bcc
POST: ent fun dgf=gm(fcc)-gm(bcc);
   ... the command in full is ENTER_SYMBOL
POST: ent fun dgl=gm(liq)-gm(bcc);
   ... the command in full is ENTER_SYMBOL
POST: ent fun dgh=gm(hcp)-gm(bcc);
   ... the command in full is ENTER_SYMBOL
POST: @@ and enter a new table and set it as y-axis
POST: ent tab g2
   ... the command in full is ENTER_SYMBOL
Variable(s): dgf dgl dgh;
POST: s-d-a y g2
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: set-title example 2b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ In order to have some identification on the lines
POST: @@ use the command SET_LABEL
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /A/:  D
POST: set-title example 2c
POST: pl
   ... the command in full is PLOT_DIAGRAM
```

```
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Now plot enthalpies
POST: ent tab h1
   ... the command in full is ENTER_SYMBOL
Variable(s): hm(bcc) hm(fcc) hm(liq) hm(hcp);
POST: s-d-a y h1
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: set-title example 2d
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ And finally plot heat capacities
POST: ent fun cpb=hm(bcc).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cpf=hm(fcc).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cpl=hm(liq).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cph=hm(hcp).t;
   ... the command in full is ENTER_SYMBOL
POST: ent tab cp1
   ... the command in full is ENTER_SYMBOL
Variable(s): t cpb cpf cpl cph;
POST: s-d-a y
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : cp1
COLUMN NUMBER /*/:  2-5
POST: s-d-a x cp1 1
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 2e
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@
POST: @@ In the next case plot functions for a binary system
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: go d
   ... the command in full is GOTO_MODULE
TDB_SSOL2: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 B2_BCC                 L12_FCC                AL5FE4:
   REJECTED
 GAS:G                  AQUEOUS:A              WATER:A
   REJECTED
 REINITIATING GES5 .....
TDB_SSOL2: @@ select the Cu-Fe system and only
TDB_SSOL2: @@ the fcc, bcc, liquid and hcp phases
TDB_SSOL2: d-sys fe cu
   ... the command in full is DEFINE_SYSTEM
 FE                     CU  DEFINED
TDB_SSOL2: rej ph /all
   ... the command in full is REJECT
 LIQUID:L               FCC_A1                 BCC_A2
 HCP_A3                 CBCC_A12               CUB_A13
 FE4N                   CUZN_EPS               ALCU_EPSILON
 ALCU_ETA  REJECTED
TDB_SSOL2: rest ph fcc bcc liq hcp
   ... the command in full is RESTORE
 FCC_A1                 BCC_A2                 LIQUID:L
 HCP_A3  RESTORED
TDB_SSOL2: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:  CONSTITUENT
 LIQUID:L    :CU FE:
```

```
 > Liquid solution, mainly metallic but also with CaO-SiO2
FCC_A1      :CU FE:VA:
 > This is also the MC(1-x) carbide or nitride
BCC_A2      :CU FE:VA:
HCP_A3      :CU FE:VA:
 > This is also the M2C carbide and M2N nitride
TDB_SSOL2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
   'A. Jansson, Report D 73, Metallografi, KTH, (1986); CU-FE'
   'Unassessed parameter, inserted to make this phase less stable.'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
       September 1989'
 -OK-
TDB_SSOL2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ set conditions for a single equilibrium
POLY_3: s-c t=1000,p=1e5,n=1,w(cu)=.01
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          548  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ select the fraction of Cu as axis variable
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/:  w(cu)
Min value /0/:  0
Max value /1/:  1
Increment /.025/:  .025
POLY_3: @@ Save always
POLY_3: save tcex02b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ Now a special STEP option will be selected as the NORMAL
POLY_3: @@ option would only calculate the stable phases. The option
POLY_3: @@ SEPARATE means that all entered phases will be calculated
POLY_3: @@ separately.
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  ?
 The following options are available:
 NORMAL             Stepping with given conditions
 INITIAL_EQUILIBRIA An initial equilibrium stored at every step
 EVALUATE           Specified variables evaluated after each step
 SEPARATE_PHASES    Each phase calculated separately
 T-ZERO             T0 line calculation
 PARAEQUILIBRIUM    Paraequilibrium diagram
 MIXED_SCHEIL       Scheil with fast diffusing elements
 ONE_PHASE_AT_TIME  One phase at a time
Option? /NORMAL/:  sep
 Phase Region from   0.529789     for:
     LIQUID
     BCC_A2
     FCC_A1
     HCP_A3

 Phase Region from   0.529789     for:
     LIQUID
     BCC_A2
```

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     FCC_A1
     HCP_A3
 *** Buffer saved on file *** tcex02b.POLY3
POLY_3: @@ Now plot the results in various ways
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: @@ Set the Gm of all phases on the y-axis
POST: s-d-a y gm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: @@ and the mole percent of Cu on the x-axis
POST: s-d-a x x(cu)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-p-f ##1,,,,,,
POST:
POST: set-title example 2f
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Now plot the enthalpy
POST: s-d-a y hm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: set-title example 2g
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ and finally the entropy
POST: s-d-a y sm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: set-title example 2h
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ The third case: ternary system, Fe-V-C
POST: @@ Calculate and plot Gm from the iron corner to VC
POST: ba
   ... the command in full is BACK
POLY_3: go d
   ... the command in full is GOTO_MODULE
TDB_SSOL2: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 B2_BCC                 L12_FCC                AL5FE4:
   REJECTED
 GAS:G                  AQUEOUS:A              WATER:A
   REJECTED
 REINITIATING GES5 .....
TDB_SSOL2: d-sys fe v c
   ... the command in full is DEFINE_SYSTEM
 FE                     V                      C
   DEFINED
TDB_SSOL2: rej ph / all
   ... the command in full is REJECT
 LIQUID:L               FCC_A1                 BCC_A2
 HCP_A3                 DIAMOND_A4             CBCC_A12
 CUB_A13                SIGMA                  GRAPHITE
 CEMENTITE              KSI_CARBIDE            M23C6
 M7C3                   M3C2                   V3C2
 M5C2                   FE4N                   FECN_CHI
   REJECTED
TDB_SSOL2: rest ph fcc bcc hcp liq
   ... the command in full is RESTORE
 FCC_A1                 BCC_A2                 HCP_A3
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 LIQUID:L  RESTORED
TDB_SSOL2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
   'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267
       TRITA 0237 (1984); C-FE'
   'W. Huang, TRITA-MAC 431 (1990); C-V'
   'W. Huang, TRITA-MAC 432 (Rev 1989,1990); FE-V'
   'W. Huang, TRITA-MAC 432 (1990); C-Fe-V'
   'H. Du and M. Hillert, revision; C-Fe-N'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
       September 1989'
   'J-O Andersson, CALPHAD Vol 7, (1983), p 305-315 (parameters revised
       1986 due to new decription of V) TRITA 0201 (1982); FE-V'
 -OK-
TDB_SSOL2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ set conditions for a single equilibrium
POLY_3: s-c t=1000,p=1e5,n=1,w(v)=.0015,x(c)=.001
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7434  grid points in            1  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL2

 Conditions:
 T=1000, P=1E5, N=1, W(V)=1.5E-3, X(C)=1E-3
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.57951E+01
 Total Gibbs energy -4.23955E+04,  Enthalpy  2.45653E+04,  Volume  7.28762E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.0000E-03  2.1527E-04 3.4517E-02 -2.7989E+04 SER
 FE                      9.9736E-01  9.9828E-01 6.1897E-03 -4.2278E+04 SER
 V                       1.6429E-03  1.5000E-03 4.0603E-07 -1.2236E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.9814E-01, Mass 5.5735E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  9.99368E-01  V   6.07187E-04  C   2.49236E-05

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.8638E-03, Mass 6.0522E-02, Volume fraction 1.3611E-06  Mass fractions:
 V   8.23695E-01  C   1.75506E-01  FE  7.99461E-04
POLY_3: @?<Hit_return_to_continue>
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FCC_A1#2                ENTERED    0.00000000E+00  1.86381384E-03
 BCC_A2                  ENTERED    0.00000000E+00  9.98136187E-01
 FCC_A1#1                ENTERED   -3.46201654E-02  0.00000000E+00
 HCP_A3#1                ENTERED   -2.87533368E-01  0.00000000E+00
 HCP_A3#2                ENTERED   -2.87533368E-01  0.00000000E+00
 LIQUID                  ENTERED   -6.51060211E-01  0.00000000E+00
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```
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Note we have several composition sets because fcc
POLY_3: @@ (and possibly hcp) can exist both as metallic and
POLY_3: @@ as carbide. However, in this case it is unecessary
POLY_3: @@ as we are only interested in the value of the
POLY_3: @@ thermodynamic functions, not the equilibrium, and therefore
POLY_3: @@ we suspend them
POLY_3: c-s p fcc#1 hcp#2
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:  sus
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1000, P=1E5, N=1, W(V)=1.5E-3, X(C)=1E-3
 DEGREES OF FREEDOM 0
POLY_3: @@ We would like to calculate the Gibbs energy from
POLY_3: @@ pure Fe to the corner VC. Select a line with equal
POLY_3: @@ fraction of V and C
POLY_3: s-c x(v)-x(c)=0
   ... the command in full is SET_CONDITION
POLY_3: s-c w(v)=none
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1000, P=1E5, N=1, X(C)=1E-3, X(V)-X(C)=0
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         7434  grid points in           0  s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL2

 Conditions:
 T=1000, P=1E5, N=1, X(C)=1E-3, X(V)-X(C)=0
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.57983E+01
 Total Gibbs energy -4.23417E+04,  Enthalpy  2.46252E+04,  Volume  7.29341E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.0000E-03  2.1526E-04 9.5408E-02 -1.9536E+04 SER
 FE                      9.9800E-01  9.9887E-01 6.1909E-03 -4.2277E+04 SER
 V                       1.0000E-03  9.1296E-04 1.6017E-07 -1.3010E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.9858E-01, Mass 5.5752E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  9.99692E-01  V   2.40066E-04  C   6.83772E-05

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.4209E-03, Mass 4.5815E-02, Volume fraction 1.6714E-06  Mass fractions:
 V   8.19759E-01  C   1.78955E-01  FE  1.28636E-03
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Set the fraction of C as axis
POLY_3: @@ The fraction of V will be the same
POLY_3: s-a-v
   ... the command in full is SET_AXIS_VARIABLE
Axis number: /1/:  1
Condition /NONE/:  x(c)
Min value /0/:  0
Max value /1/:  .5
Increment /.0125/:  .0125
POLY_3: save tcex02c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ step along the axis
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  sep
 Phase Region from   0.330065     for:
     LIQUID
     BCC_A2
```

```
     FCC_A1#2

 Phase Region from   0.330065     for:
     LIQUID
     BCC_A2
     FCC_A1#2

 Phase Region from   0.480604E-02 for:
     HCP_A3#1

 Phase Region from   0.480604E-02 for:
     HCP_A3#1
 *** Buffer saved on file *** tcex02c.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: @@ plot the Gm versus carbon content
POST: l-p-s
   ... the command in full is LIST_PLOT_SETTINGS
 GRAPHIC DEVICE: X-windows ( # 9)  PLOTFILE: SCREEN
 FONT:  (# 1)  Cartographic Roman
 AXIS PLOT            YES
 RASTER PLOT         : NO
 TRIANGULAR PLOT     : NO

 AUTOMATIC SCALING

 AUTOMATIC AXIS TEXT

 AXIS VARIABLES
POST: s-d-a x x(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y gm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: s-p-f ##1,,,,,,,
POST:
POST: set-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 2i
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ The fourth case: more partial derivatives
POST: back
POLY_3: go d
   ... the command in full is GOTO_MODULE
TDB_SSOL2: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 B2_BCC                  L12_FCC                 AL5FE4:
   REJECTED
 GAS:G                   AQUEOUS:A               WATER:A
   REJECTED
 REINITIATING GES5 .....
TDB_SSOL2: def-sys al cu
   ... the command in full is DEFINE_SYSTEM
 AL                      CU  DEFINED
TDB_SSOL2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
```

```
   'I Ansara, P Willemin B Sundman (1988); Al-Ni'
   'N. Saunders, unpublished research, COST-507, (1991); Al-Cu'
   'M. Kowalski, RWTH, unpublished work (1990); Cu-Zn'
   'N. Saunders, private communication (1991); Al-Ti-V'
 BINARY L0 PARAMETERS ARE MISSING
 CHECK THE FILE MISSING.LIS FOR COMPLETE INFO
 -OK-
TDB_SSOL2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1400 p=1e5 n=1 x(al)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1242  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL2

 Conditions:
 T=1400, P=1E5, N=1, X(AL)=0.1
 DEGREES OF FREEDOM 0

 Temperature   1400.00 K (  1126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.98896E+01
 Total Gibbs energy -8.50789E+04,  Enthalpy  3.56307E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      1.0000E-01  4.5052E-02 1.5146E-06 -1.5598E+05 SER
 CU                      9.0000E-01  9.5495E-01 1.3173E-03 -7.7201E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.9890E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  9.54948E-01  AL  4.50522E-02
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ check the activity of aluminum
POLY_3: show acr(al)
   ... the command in full is SHOW_VALUE
 ACR(AL)=1.5146067E-6
POLY_3: @@ This activity value is referred to fcc Al at 298.15 K.
POLY_3: @@ Set proper reference state for activities
POLY_3: set-ref-state al
   ... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature /*/:
Pressure /1E5/:
POLY_3:
POLY_3: set-ref-state cu
   ... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature /*/:
Pressure /1E5/:
POLY_3:
POLY_3: show acr(al)
   ... the command in full is SHOW_VALUE
 ACR(AL)=9.0463987E-4
POLY_3: @@ This value is better.  The corresponding chemical potential is
POLY_3: show mur(al)
   ... the command in full is SHOW_VALUE
 MUR(AL)=-81575.013
POLY_3: @@ The relation is simply that acr(al)=exp(mur(al)/RT).  Check that
POLY_3: enter fun test
   ... the command in full is ENTER_SYMBOL
Function: exp(mur(al)/8.31451/T);
POLY_3: show test
   ... the command in full is SHOW_VALUE
 TEST=9.0463987E-4
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ POLY allows calculation of partial derivatives of thermodynamic
POLY_3: @@ quantities of original reference state with respect to fractions
```

```
POLY_3: @@ that are conditions. For example
POLY_3: show gm.x(al)
   ... the command in full is SHOW_VALUE
 GM.X(AL)=-78783.802
POLY_3: @@ This is not the same as the chemical potential. It actually
POLY_3: @@ equals to the so-called diffusion potential: mu(al)-mu(cu).
POLY_3: ent fun diffmu=mu(al)-mu(cu);
   ... the command in full is ENTER_SYMBOL
POLY_3: show diffmu
   ... the command in full is SHOW_VALUE
 DIFFMU=-78783.802
POLY_3: @@ The relation between the chemical potential and the partial derivative is
POLY_3: @@
POLY_3: @@ mu(al) = gm + gm.x(al) - x(al)*gm.x(al)
POLY_3: @@
POLY_3: @@ We can enter this as a function also.
POLY_3: enter fun dgdx=gm+gm.x(al)-x(al)*gm.x(al);
   ... the command in full is ENTER_SYMBOL
POLY_3: sh dgdx
   ... the command in full is SHOW_VALUE

 Warning: All functions are evaluated for this command and as there are
 one or more functions with a derivative which may be irrelevant
 for this equilibrium some functions may have wrong values.
 If possible enter derivatives as VARIABLES instead

 DGDX=-155984.34
POLY_3: sh mu(al)
   ... the command in full is SHOW_VALUE
 MU(AL)=-155984.34
POLY_3: @@ Partial entropy is the negative of mu(al).t
POLY_3: ent fun ps=-mu(al).t;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh ps
   ... the command in full is SHOW_VALUE

 Warning: All functions are evaluated for this command and as there are
 one or more functions with a derivative which may be irrelevant
 for this equilibrium some functions may have wrong values.
 If possible enter derivatives as VARIABLES instead

 PS=93.397812
POLY_3: @@ Partial enthalpy is h = g + s*t
POLY_3: enter fun ph=mu(al)+ps*t;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh ph
   ... the command in full is SHOW_VALUE

 Warning: All functions are evaluated for this command and as there are
 one or more functions with a derivative which may be irrelevant
 for this equilibrium some functions may have wrong values.
 If possible enter derivatives as VARIABLES instead

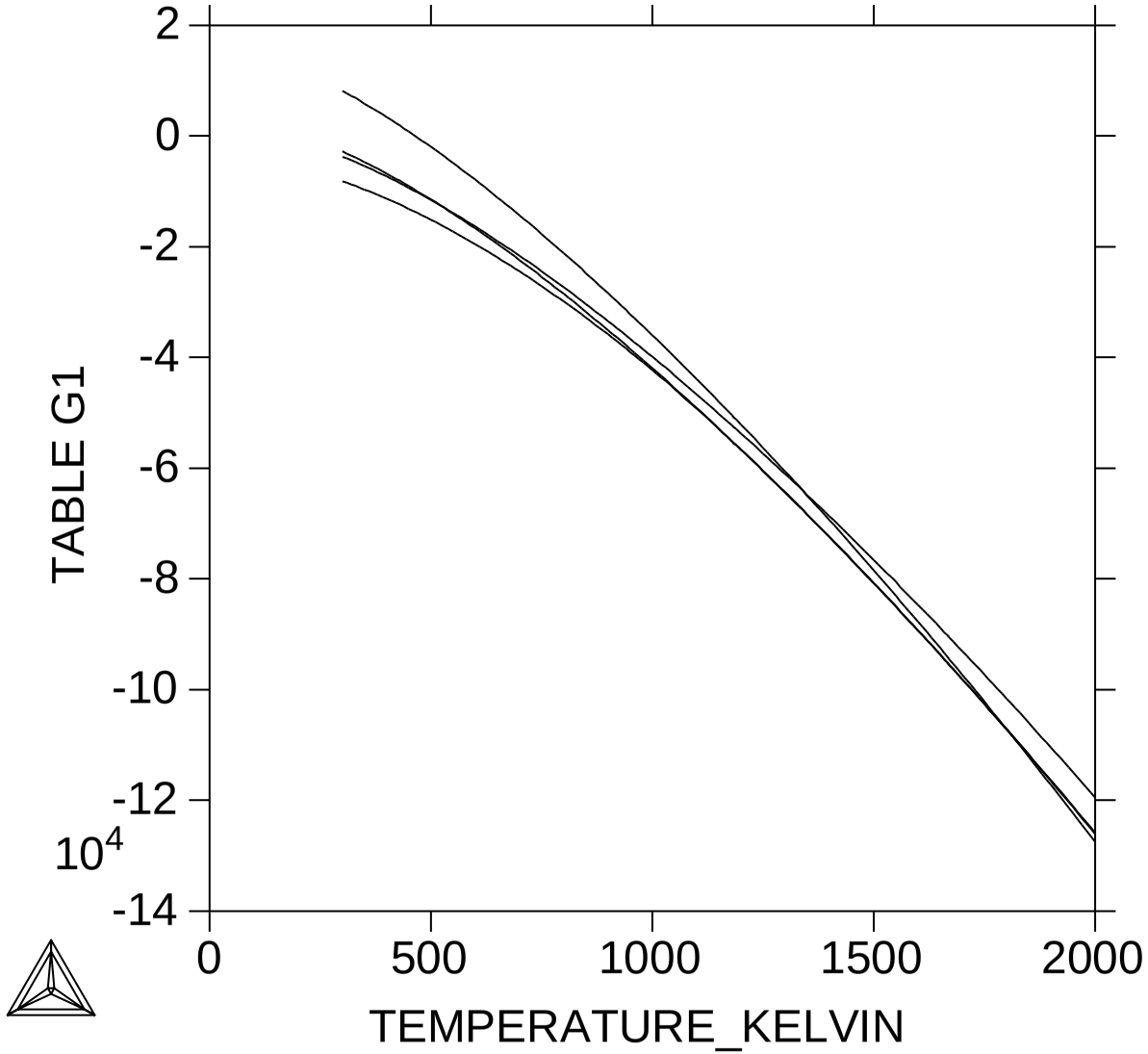
 PH=-25227.4
POLY_3: @@ Partial enthalpy can also be calculated in a similar way as chemical
POLY_3: @@ potential
POLY_3: @@ partial enthalpy = hm + hm.x(al) - x(al)*hm.x(al)
POLY_3: ent fun ph1=hm+hm.x(al)-x(al)*hm.x(al);
   ... the command in full is ENTER_SYMBOL
POLY_3: sh ph1
   ... the command in full is SHOW_VALUE

 Warning: All functions are evaluated for this command and as there are
 one or more functions with a derivative which may be irrelevant
 for this equilibrium some functions may have wrong values.
 If possible enter derivatives as VARIABLES instead

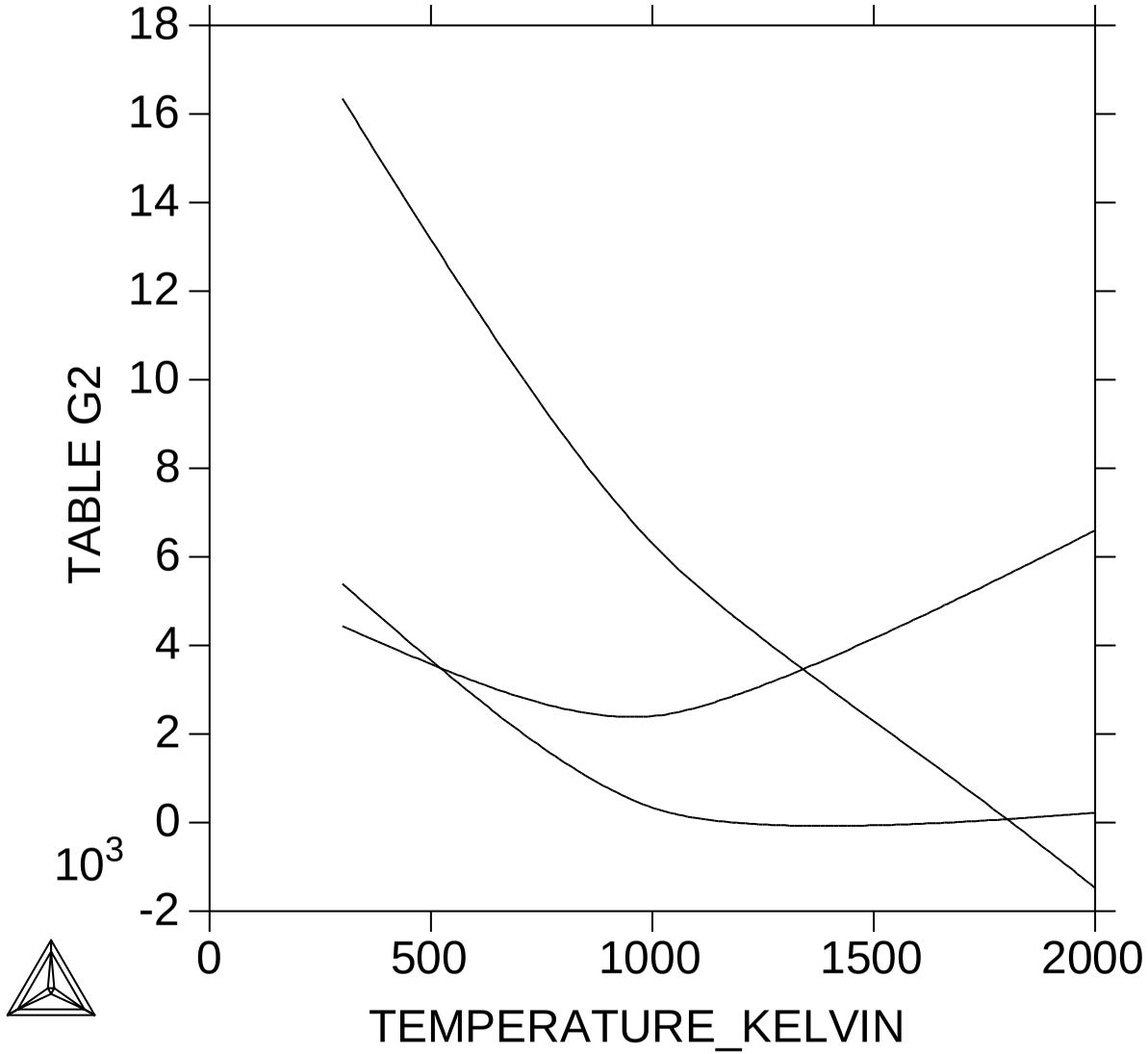
 PH1=-25227.4
POLY_3: @@ As can be seen, ph1 = ph.
POLY_3: @@ Another useful quantity is mu(al).x(al).  That is related to
POLY_3: @@ the thermodynamic factor and part of the diffusion coefficient.
POLY_3: show mu(al).x(al)
   ... the command in full is SHOW_VALUE
 MU(AL).X(AL)=307908.74
```

POLY_3: **@?<Hit_return_to_continue>**
 CPU time   2 seconds

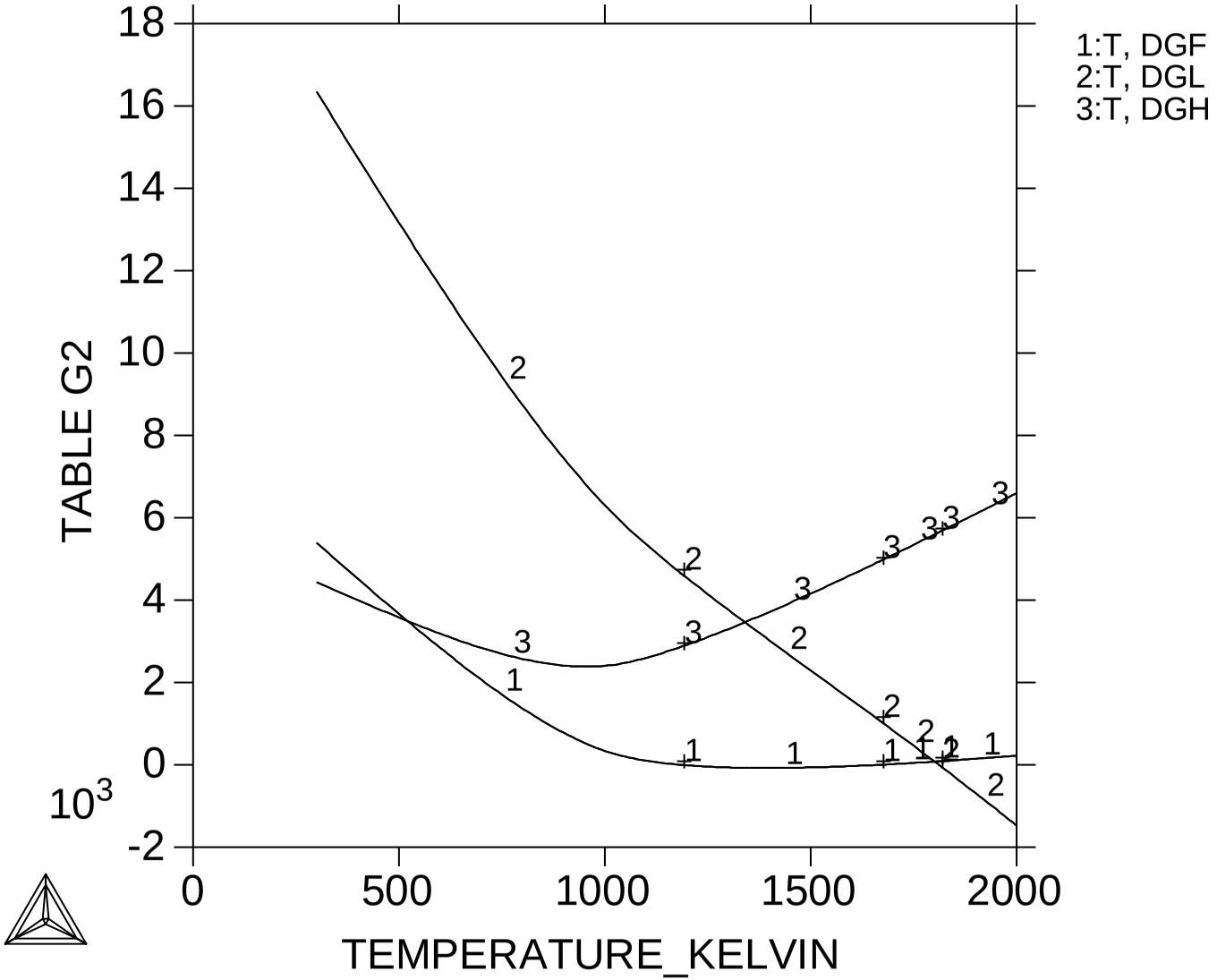
THERMO-CALC (2009.04.29:14.08) :example 2a
DATABASE:SSOL2
P=1E5, N=1



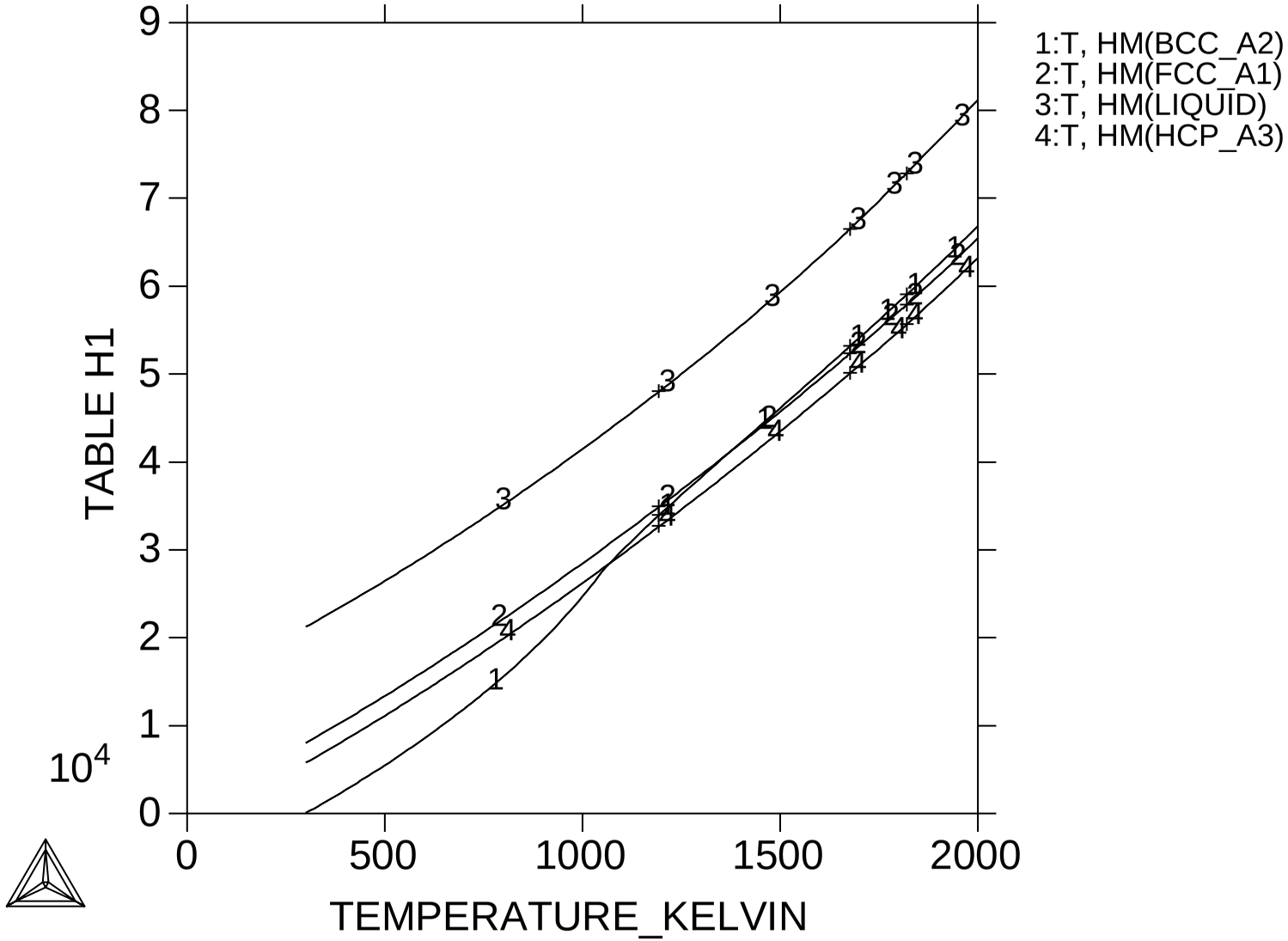
THERMO-CALC (2009.04.29:14.08) :example 2b
DATABASE:SSOL2
P=1E5, N=1



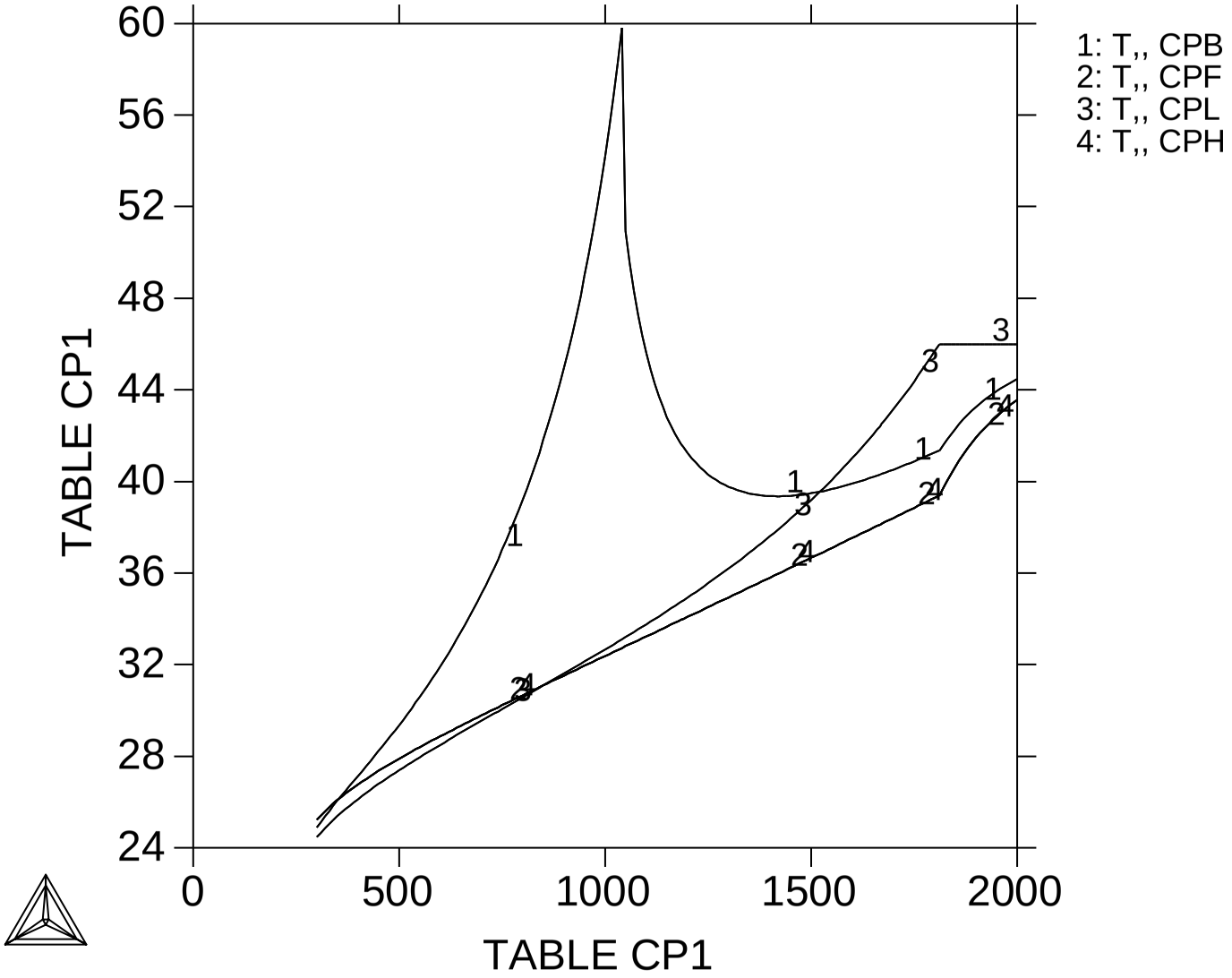
THERMO-CALC (2009.04.29:14.08) :example 2c
DATABASE:SSOL2
P=1E5, N=1



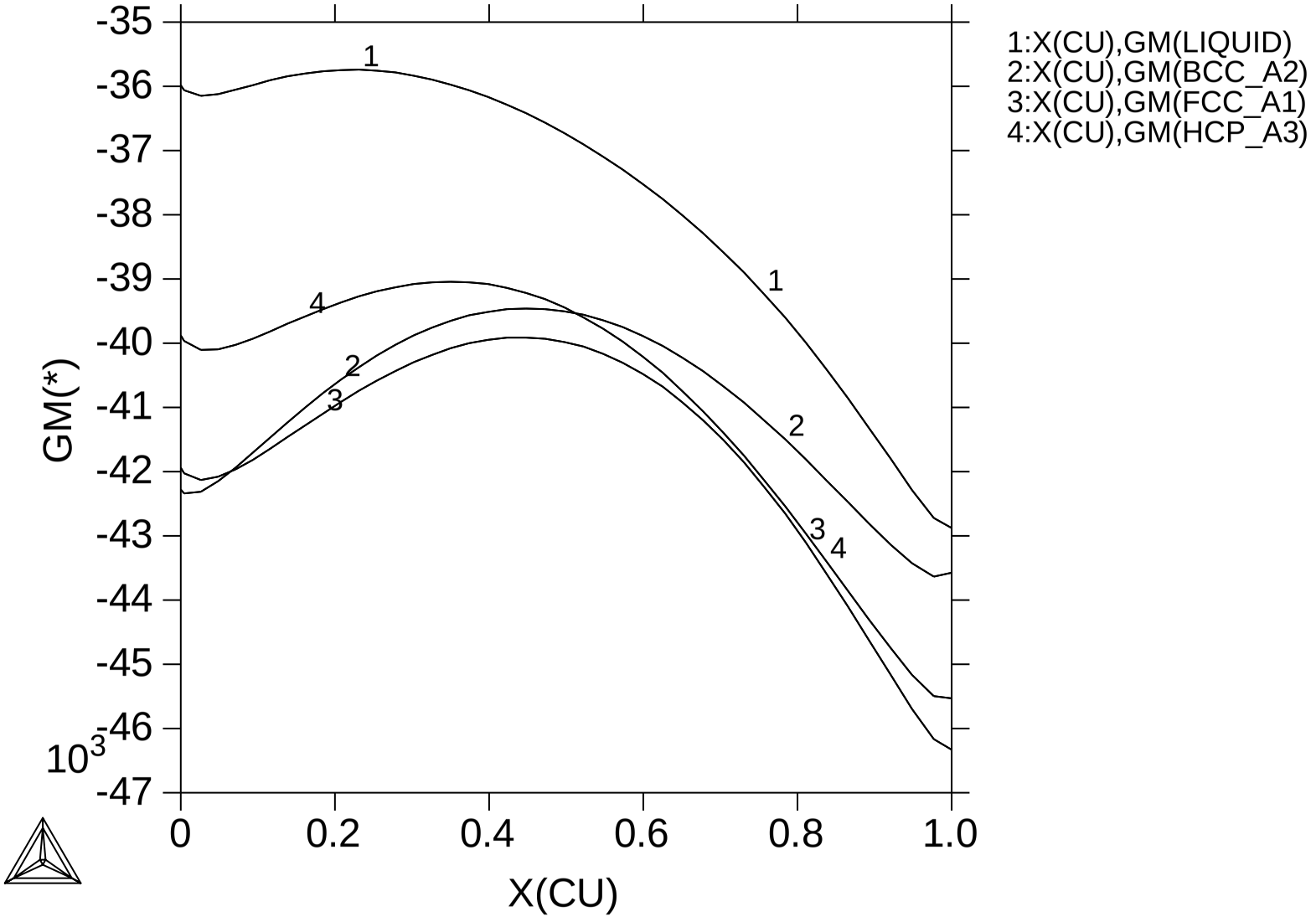
THERMO-CALC (2009.04.29:14.08) :example 2d
DATABASE:SSOL2
P=1E5, N=1



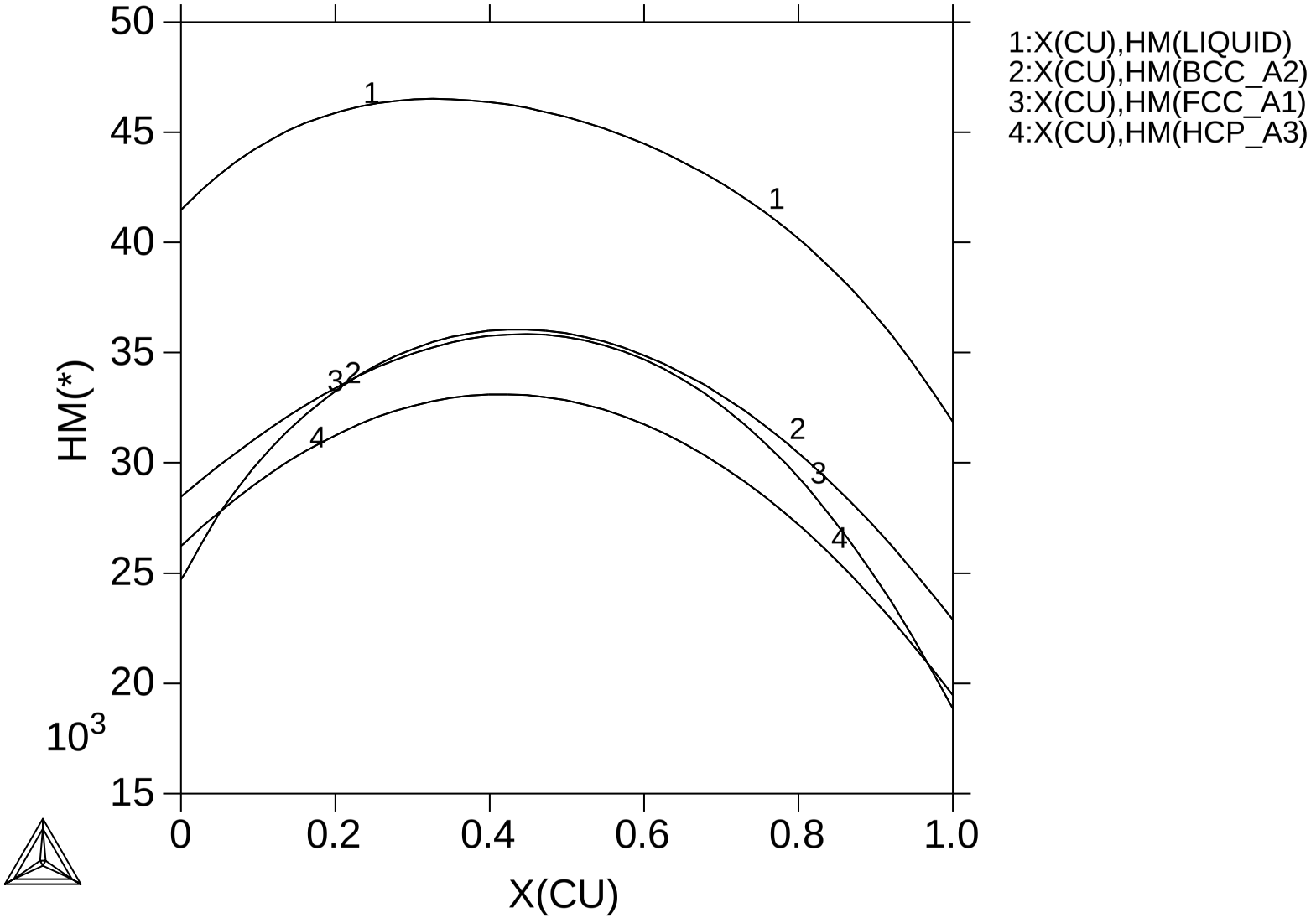
THERMO-CALC (2009.04.29:14.08) :example 2e
DATABASE:SSOL2
P=1E5, N=1



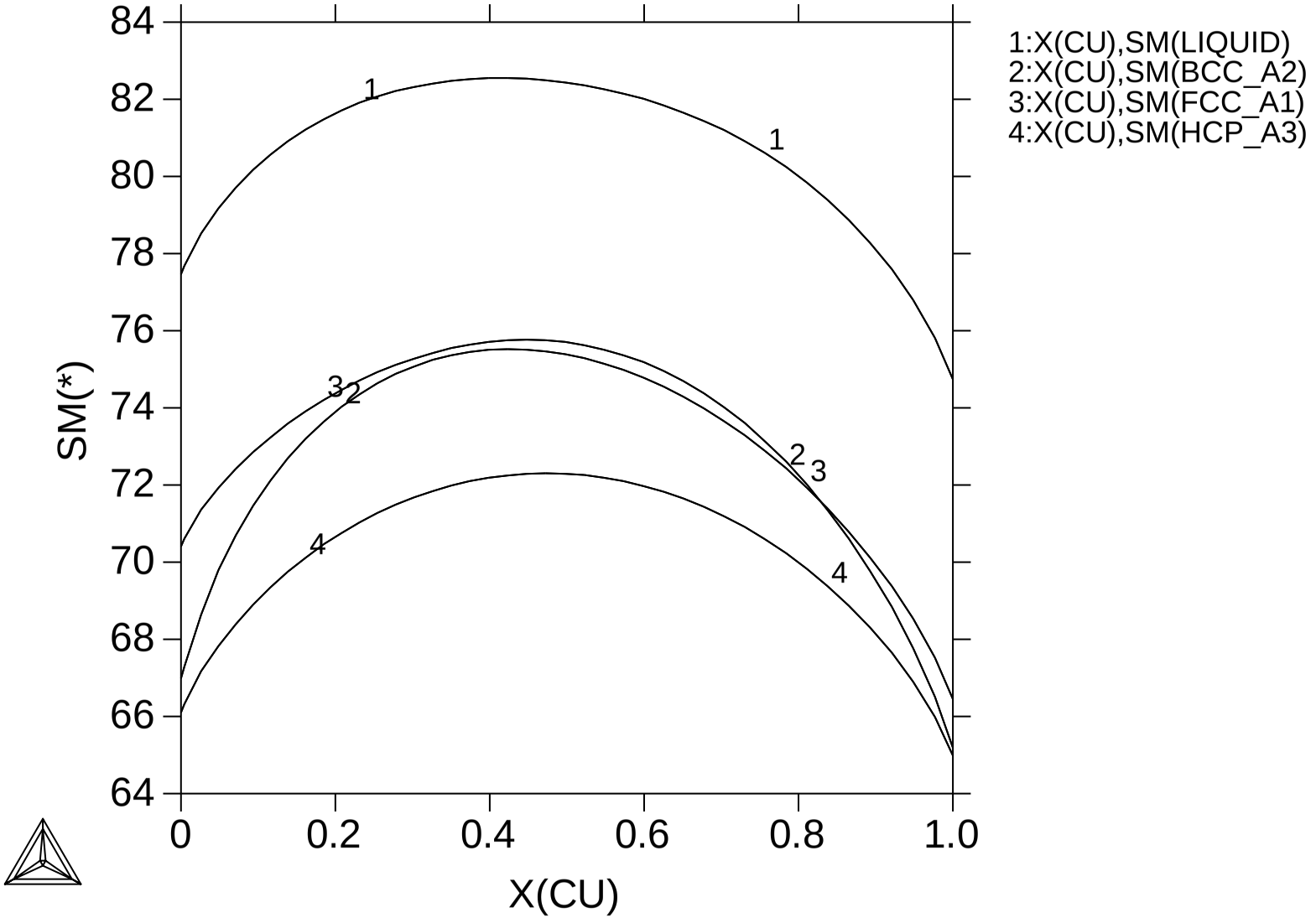
THERMO-CALC (2009.04.29:14.08) :example 2f
DATABASE:SSOL2
T=1000, P=1E5, N=1;



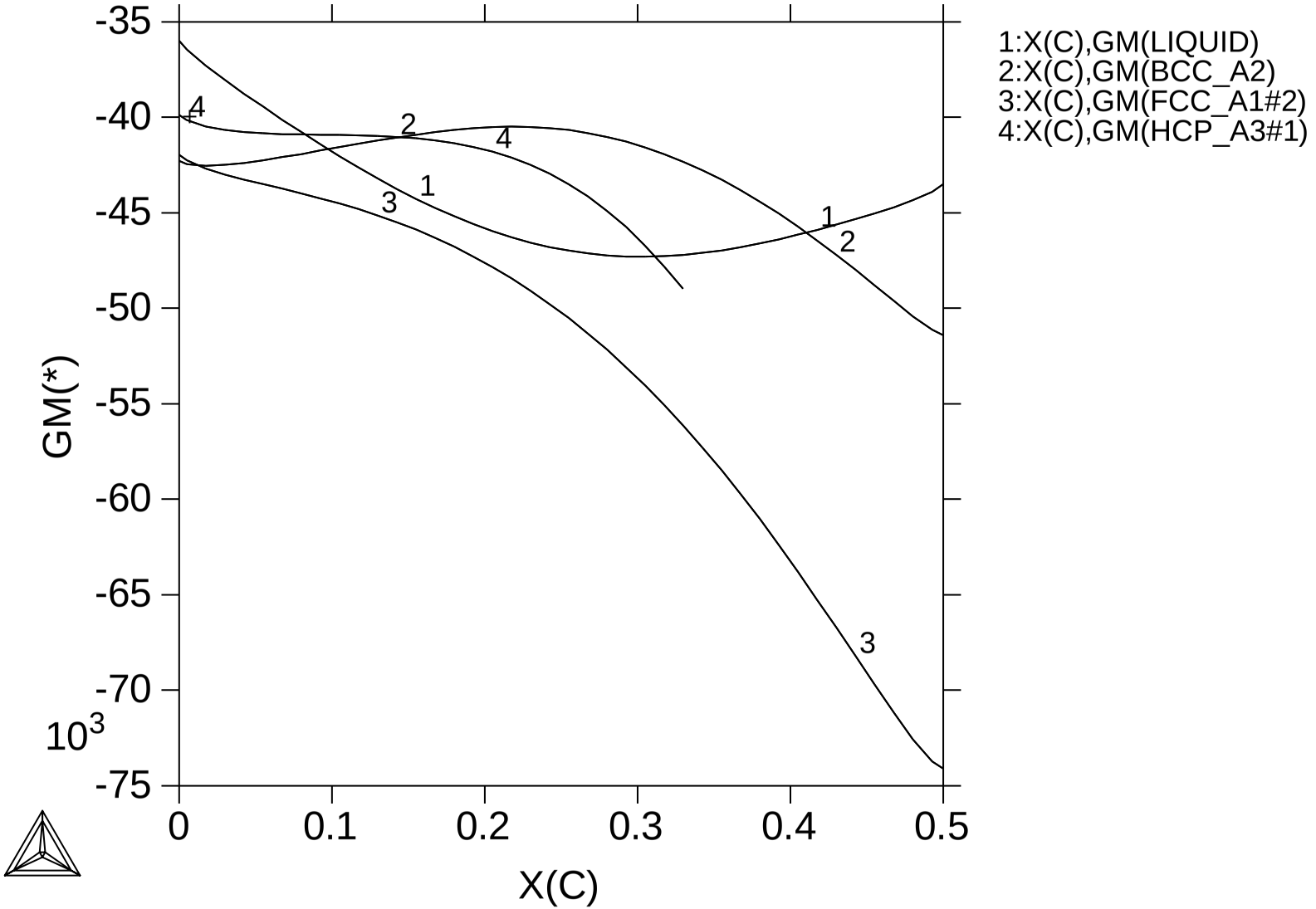
THERMO-CALC (2009.04.29:14.08) :example 2g
DATABASE:SSOL2
T=1000, P=1E5, N=1;



THERMO-CALC (2009.04.29:14.08) :example 2h
DATABASE:SSOL2
T=1000, P=1E5, N=1;



THERMO-CALC (2009.04.29:14.08) :example 2i
DATABASE:SSOL2
T=1000, P=1E5, N=1, X(V)-X(C)=0;



1:X(C),GM(LIQUID)
2:X(C),GM(BCC_A2)
3:X(C),GM(FCC_A1#2)
4:X(C),GM(HCP_A3#1)

3

Calculation of an isothermal section using the TERNARY module

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of an isothermal section using ternary module
SYS: @@
SYS: set-log ex03,,
SYS:
SYS: go tern
   ... the command in full is GOTO_MODULE

 Quick ternary phase diagram calculation module

 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
Database: /PTERN/: PTERN
First element: ?
 The following assessed systems
    AL-MG   AL-SI   MG-SI   C-FE   C-CR   C-V   CR-FE   FE-V   AL-MG-SI
  C-CR-FE   C-FE-V

First element: fe
Second element: c
Third element: cr
Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/: Phase_Diagram
Temperature (C) /1000/: 1200
Global minimization on: /Y/:
 VA  DEFINED
 REINITIATING GES5 .....
 C                       CR                      FE
   DEFINED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
  'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
       C-FE'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
      (1986); CR-FE'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
      Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'
  'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'W. Huang, TRITA-MAC 441 (1990), Fe-Mn-V-C '
 -OK-
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
 Start points provided by database
 Version S mapping is selected
```

```
 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Working hard

 Phase region boundary   1 at:   4.083E-01  4.852E-01
     BCC_A2#1
  ** M23C6
 *** Buffer saved on file: ISOTHER.POLY3
 Calculated           60  equilibria

 Phase region boundary   2 at:   4.083E-01  4.852E-01
     BCC_A2#1
  ** M23C6
 Calculated.            6  equilibria

 Phase region boundary   3 at:   3.630E-01  5.301E-01
     BCC_A2#1
  ** FCC_A1#2
  ** M23C6

 Phase region boundary   4 at:   2.107E-01  7.727E-01
     BCC_A2#1
  ** FCC_A1#1
 Calculated           28  equilibria

       :
       :
       :

 Phase region boundary  23 at:   3.630E-01  5.301E-01
     BCC_A2#1
  ** M23C6
 Calculated           61  equilibria

 Phase region boundary  24 at:   9.314E-02  2.569E-01
  ** GRAPHITE
     M7C3
 Calculated.           19  equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   4.605E-02  3.289E-01
     CEMENTITE
  ** GRAPHITE
 Calculated.            1  equilibria
 Terminating at known equilibrium

 Phase region boundary  26 at:   1.392E-01  5.858E-01
     CEMENTITE
  ** M7C3
 Calculated.            3  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: ISOTHER.POLY3
 CPU time for mapping           2  seconds

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST:
POST: @@ The plot device is set interactively
POST: @#1Plotformat
POST:
```

POST: **s-p-f ##1,,,,,**
POST:
POST: **set-title example 3a**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ Add some labels***
POST: **add .35 .3**
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in   0 s
 Calculated POLY solution   0 s, total time   0 s
 Stable phases are: GRAPHITE+M7C3
Text size: /.3999999762/:
POST: **add .05 .2**
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in   0 s
 Calculated POLY solution   0 s, total time   0 s
 Stable phases are: FCC_A1+M7C3
Text size: /.3999999762/:
POST: **set-title example 3b**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **add .3 .01**
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in   0 s
 Calculated POLY solution   0 s, total time   0 s
 Stable phases are: LIQUID+GRAPHITE
Text size: /.3999999762/:
POST: **add .35 .1**
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in   0 s
 Calculated POLY solution   0 s, total time   0 s
 Stable phases are: CEMENTIT+GRAPHITE+M7C3
Text size: /.3999999762/:
POST: **add .01 .5**
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in   0 s
 Calculated POLY solution   0 s, total time   0 s
 Stable phases are: BCC_A2+M23C6
Text size: /.3999999762/:
POST: **set-title example 3c**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ We can try the same exercise as in example 1, use***
POST: ***@@ carbon activity as one axis***
POST: **s-d-a x ac c**

... the command in full is SET_DIAGRAM_AXIS
POST: **set-title example 3d**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ With these axes it is better to have a square diagram!***
POST: **s-dia-type**
... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM (Y OR N) /N/: **N**
CREATE TETRAHEDRON WRML FILE (Y OR N) /N/:
POST:
POST: **set-title example 3e**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ The activity axis is probably better as logarithmic***
POST: **s-a-ty x**
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: **log**
POST: **set-title example 3f**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ In order for pure graphite to have activity one, the reference***
POST: ***@@ state of C should be set to graphite. In addition,***
POST: ***@@ the solubility lines now cross! Is the diagram wrong?***
POST: ***@@ No, in this case one should not use the mole fraction of Cr***
POST: ***@@ but the metallic fraction. This can be set by setting***
POST: ***@@ the status of C to "special". All species set as special***
POST: ***@@ will be excluded from the summation of fractions.***
POST: ***@@ The special status is set in the POLY module***
POST: **ba**
... the command in full is BACK
SYS: **go p-3**
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: **s-r-s**
... the command in full is SET_REFERENCE_STATE
Component: **C**
Reference phase: **gra**
Temperature /*/:
Pressure /1E5/:
POLY_3: **ch-st**
... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/: **C**
Name(s): **C**
Status: /ENTERED/: **?**
Status

The new status to be assigned must be given.

* For species, the values ENTERED or SUSPENDED can be used.

* For components, the status ENTERED, SUSPENDED or SPECIAL can be given.
SPECIAL means that this component will be excluded from sums for
mole fractions and mass fractions.

* For phases, the status ENTERED, SUSPENDED, DORMANT or FIXED can be given.
DORMANT means the same as suspended but the driving force will be
calculated. FIXED means that it is a condition that the phase is
stable at a certain amount.

Note that only component(s) may have the status SPECIAL, which implies
that they will not be included in summations for mole or mass fractions.
For instance, for the so-called "u" fractions or other normalized fractions,
when one or more of the components are excluded from the summation, one
must specify which component(s) should be excluded from the calculation
of mole or mass fraction. This component status is particularly useful

when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status SPECIAL. This is assigned by the CHANGE_STATUS command. For example, to obtain the metallic fraction in a system with as an intersitial component, one can set the component status for carbon as SPECIAL:

Change_status comp C=**special**

Important Note: Special attentions should be paid when specifying a FIXED phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below:

* The phase amount variables, NP(phase), BP(phase) and VP(phase), as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, one can use the CHANGE_STATUS command to set a relevant condition, e.g., CHANGE_STATUS phase <phase>=fix <amount> where the fixed <amount> is roughly the same as the F-suffixed quantity "NPF(phase)".

* The "NPF(phase)" quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other F-suffixed state variables [e.g., GF(phase), HF(phase) and DGF(phase)] can not be directly applied in any POLY command, implying that it can not be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, one should instead use a properly-entered symbol (function or variable), for instance,

```
      NPFabc = NP(abc)/NA
  or  NPFabc = NPM(abc)/NA*N
```

  N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy).

  For instance, the SIGMA, FCC, BCC and LIQUID phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modeled by certain models, and their NA values must be evaluated in different ways, as described below:

```
  LIQUID     (C,Cr,CrO3/2,Fe,FeO,FEO3/2,N,Ni,NiO)1  --> NA = 1
  FCC_A1     (Cr,Fe,Ni)1(Va,C,N,O)1                 --> NA = 1
  BCC_A2     (Cr,Fe,Ni)1(Va,C,N,O)3                 --> NA = 1
  SIGMA      (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18              --> NA = 30
```

  If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase has been modeled by the Two-Sublattice Ionic Liquid Model, i.e.,

```
  IONIC_LIQ  (Cr+3,Fe+2,Ni+2)p(VA,C,N,O-2,FEO3/2)q
```

  the evaluation of its NA value becomes even more complicated,

```
  NA = p+q*y(C_2ndSite)+q*(N_2ndSite)+q*(O-2_2ndSite)+q*(FeO3/2_2ndSite)
```

  where the stoichiometric coefficients p and q are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by multiple-sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.

* Obviously, there will be no strange thing when using a zero value [i.e., 0] in a FIXED phase-status, since it simply means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e., it just starts becoming stable on one side of a corresponding phase-boundary line or unstable on the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states.

* However, when a non-zero value [it must always be positive; e.g., 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific FIXED-status phase in a calculated equilibrium state any longer; instead, the <equilibrium amount> value is the "NPF(phase)" value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations.

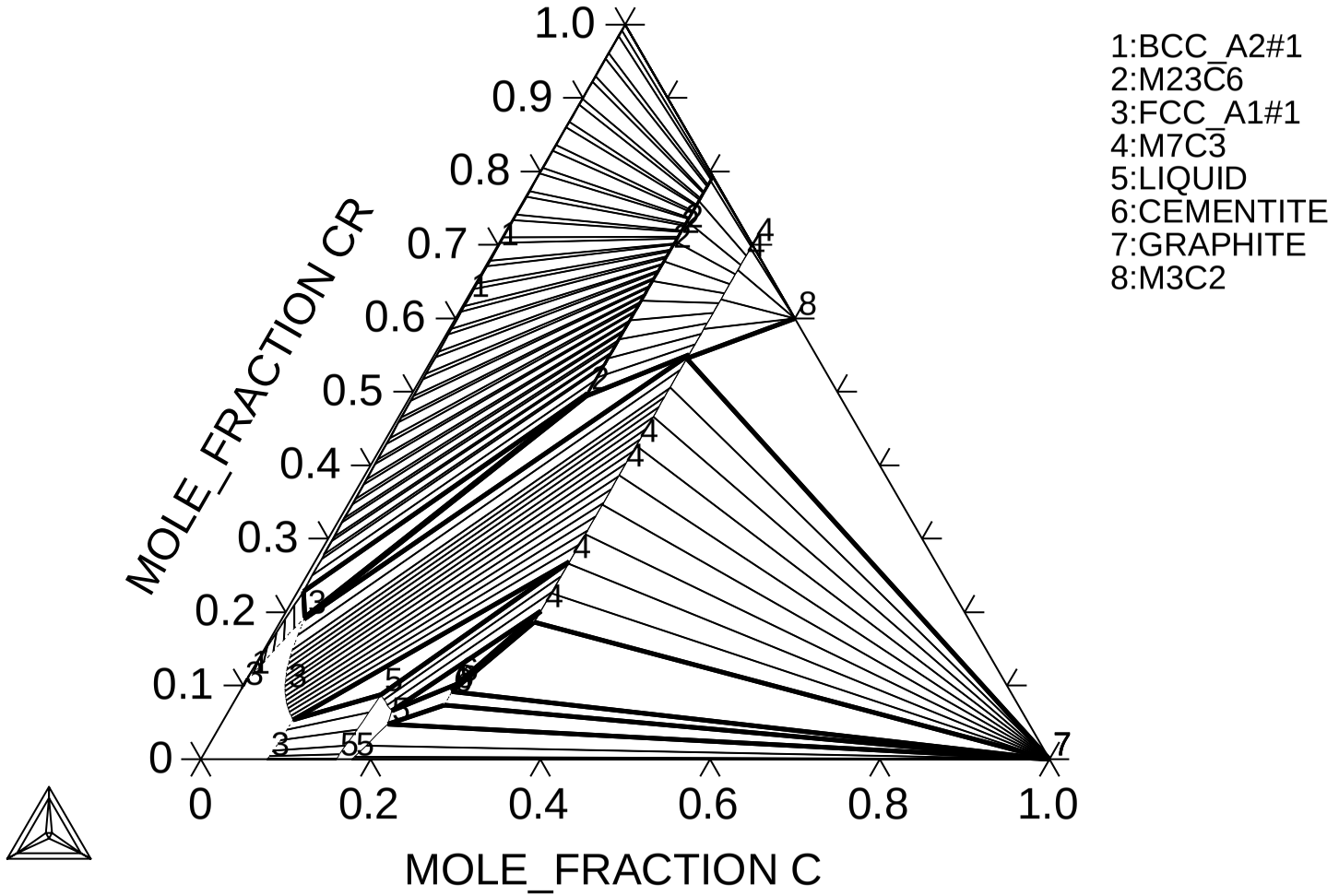
  Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase has been predefined

as a single-sublattice solution phase (such as metallic liquid phase
in multicomponent alloy systems) and the total system size as one mole
(i.e., N=1).

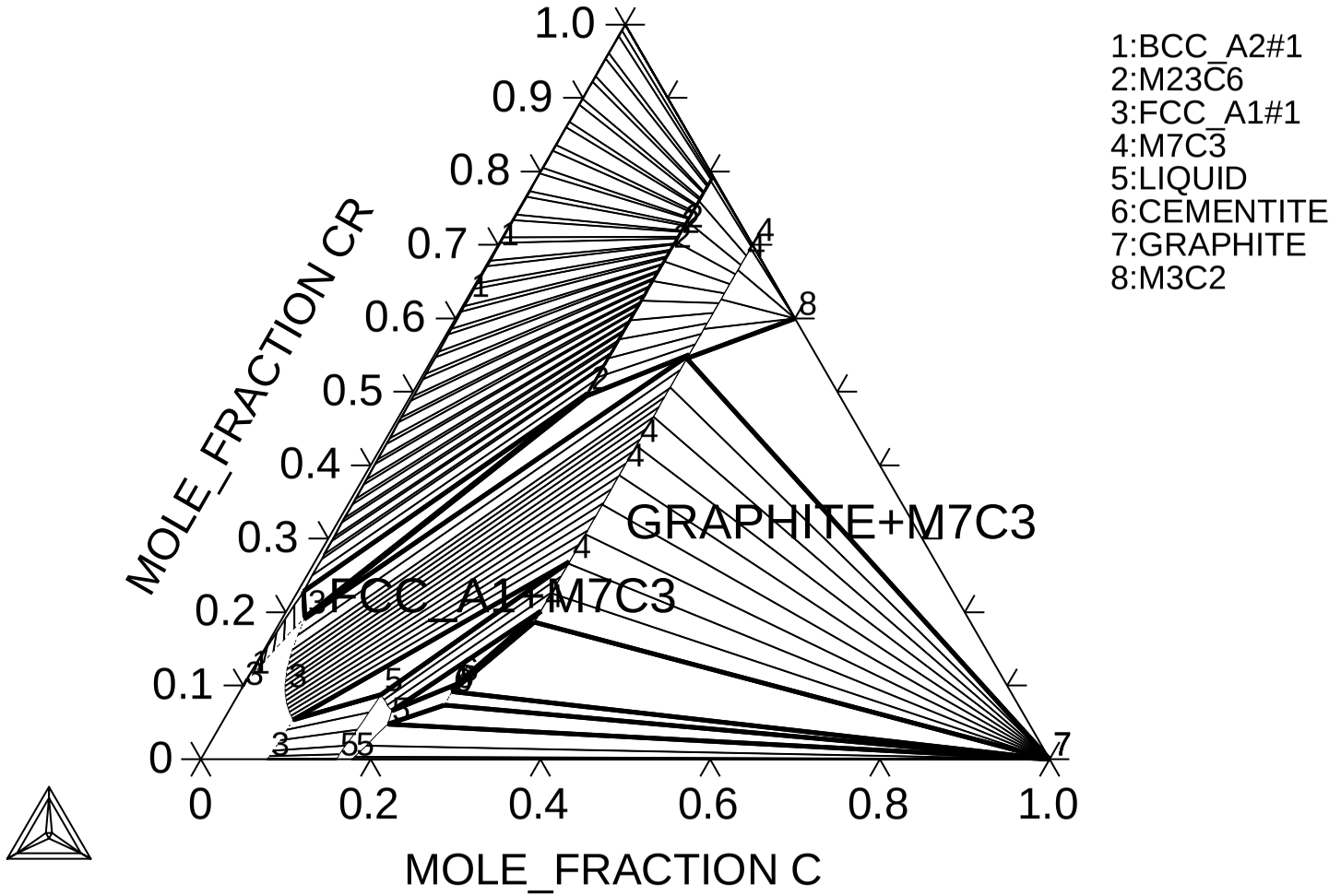
When a phase is described by a solution model in which two or more
sublattices are considered and these sublattice sites may also have
different stoichiometric coefficients [meaning that the mixture phase
could have more than one atom in formula [NA>1; see some examples above],
the unity value should not be used when setting the FIXED status for
the phase; instead, one should use an appropriate value that ranges
from 0 to a "NPF(phase)" value that equals to or is smaller than 1/NA
(if the total system size N=1) or 1/NA*N (if N differs from unity).
For this reason, if a multicomponent system bears an IONIC_LIQUID phase
that is described by the Two-Sublattice Ionic Liquid Model (or any
other multiple-sublattice ionic solution phases), it is very difficult
to use a proper "NPF(ION_LIQ)" value in setting its FIXED phase-status,
because that should be less than (or equal to) the complex value of
N/[p+q*y(C_2ndSite)+q*(N_2ndSite)+q*(O-2_2ndSite)+q*(FeO3/2_2ndSite)].

Status: /ENTERED/: special
POLY_3:
POLY_3: **post**
POST: **s-p-f ##1,,,,,**
POST:
POST: **set-title example 3g**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ Finally scale***
POST: **s-s x n .001 1**
   ... the command in full is SET_SCALING_STATUS
POST: **set-title example 3h**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ This kind of diagram is useful to understand diffusion paths.***
POST: ***@@***
POST: ***@@ The phase labels were lost when we changed axis***
POST: ***@@ One may add them again***
POST: **add .05 .3**
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
 Calculated   7985 grid points in   0 s
 Stable phases are: FCC_A1+M7C3
Text size: /.3999999762/:
POST: **set-title example 3i**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
 CPU time   5 seconds

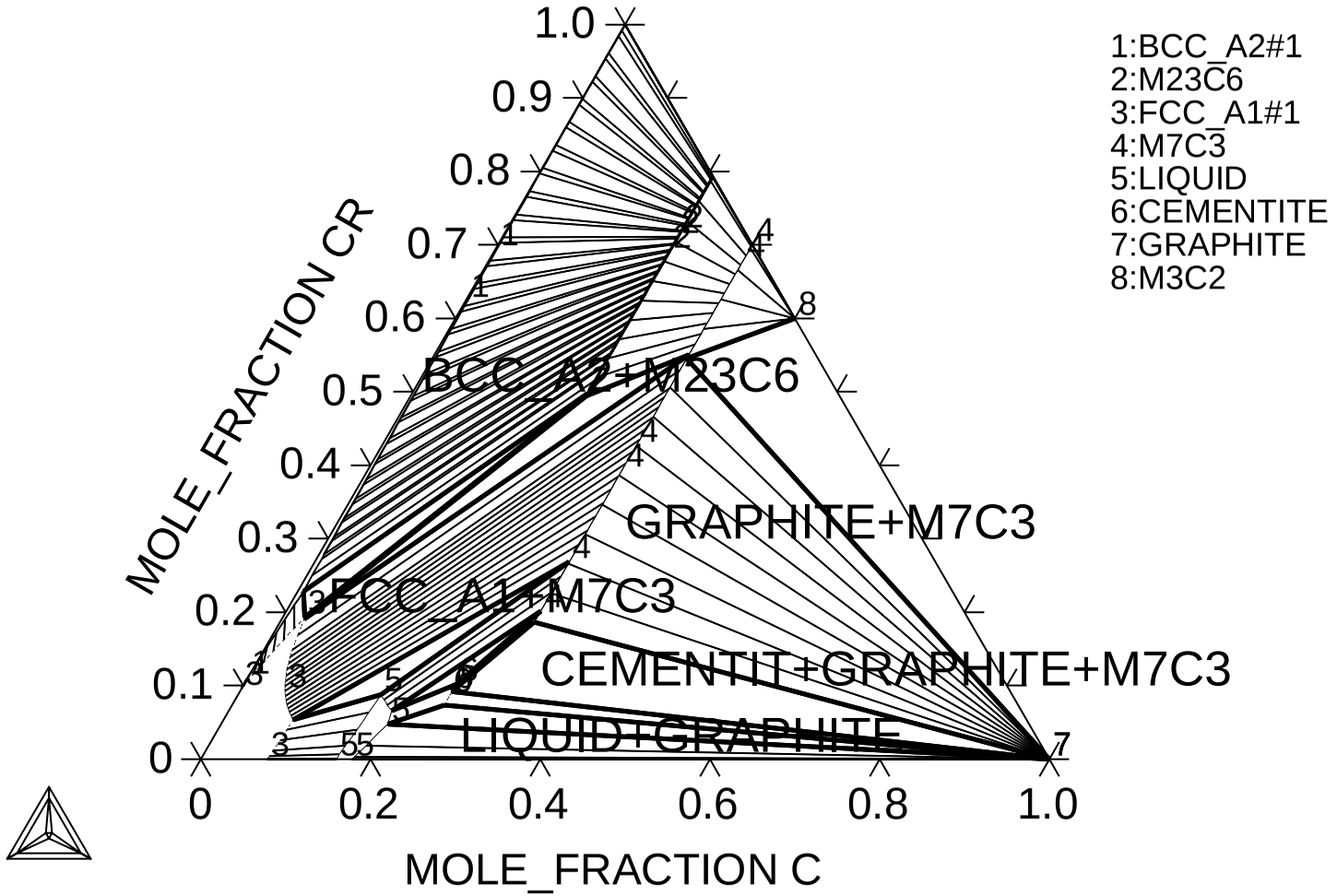
THERMO-CALC (2009.04.29:14.08) :example 3a
DATABASE:PTERN
T=1473.15, P=1E5, N=1;



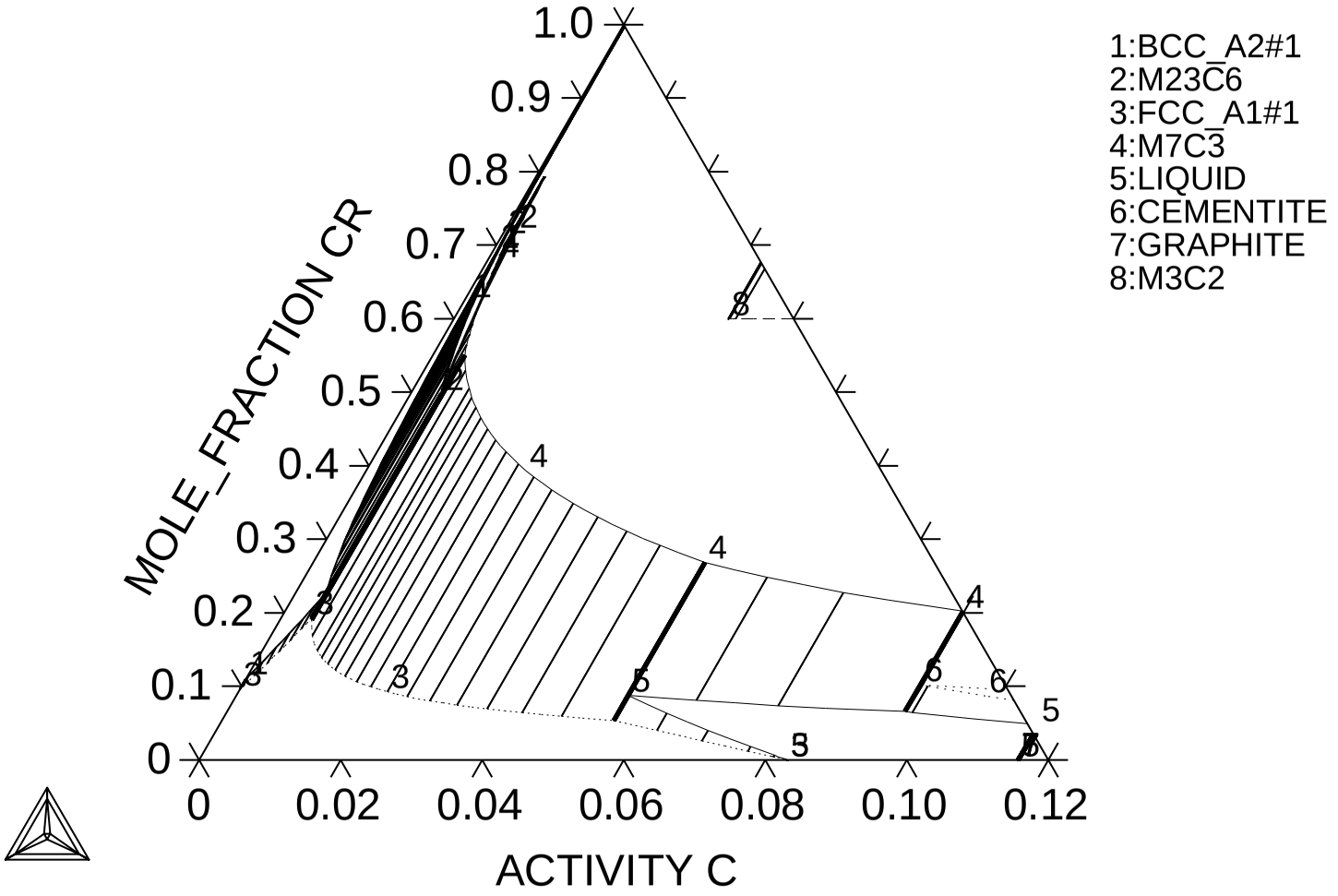
THERMO-CALC (2009.04.29:14.08) :example 3b
DATABASE:PTERN
T=1473.15, P=1E5, N=1;



THERMO-CALC (2009.04.29:14.08) :example 3c
DATABASE:PTERN
T=1473.15, P=1E5, N=1;

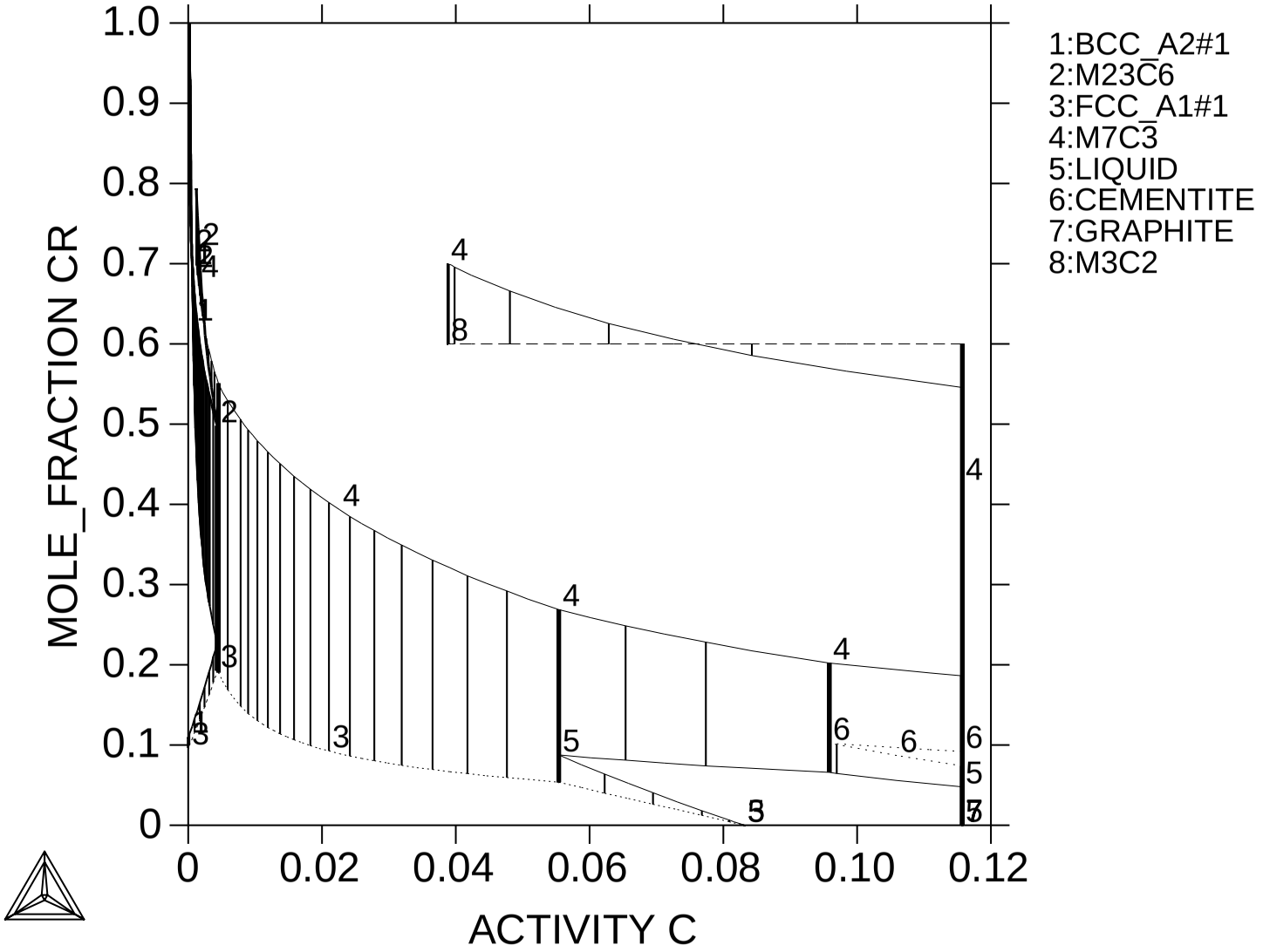


THERMO-CALC (2009.04.29:14.08) :example 3d
DATABASE:PTERN
T=1473.15, P=1E5, N=1;

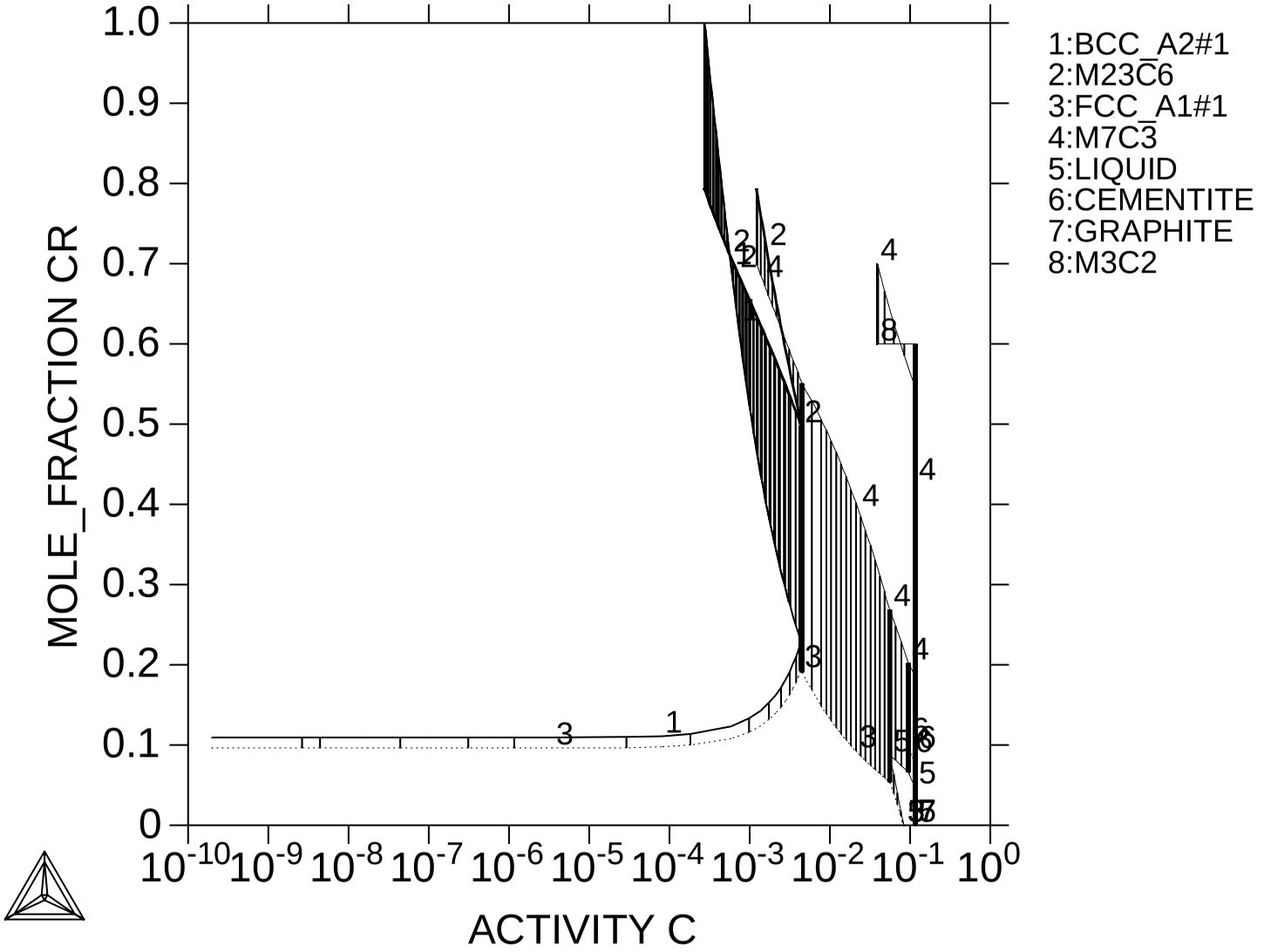


1:BCC_A2#1
2:M23C6
3:FCC_A1#1
4:M7C3
5:LIQUID
6:CEMENTITE
7:GRAPHITE
8:M3C2

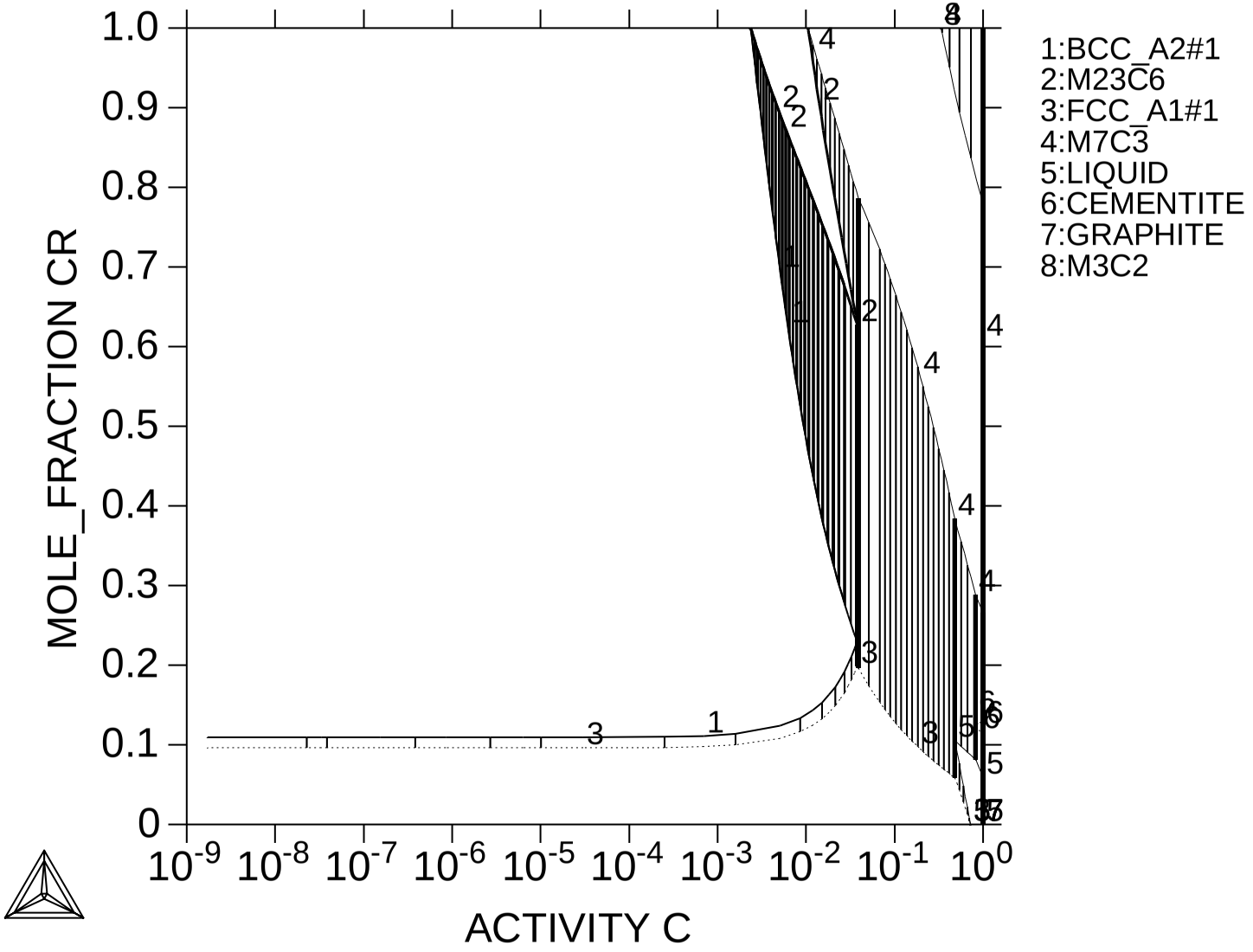
THERMO-CALC (2009.04.29:14.08) :example 3e
DATABASE:PTERN
T=1473.15, P=1E5, N=1;



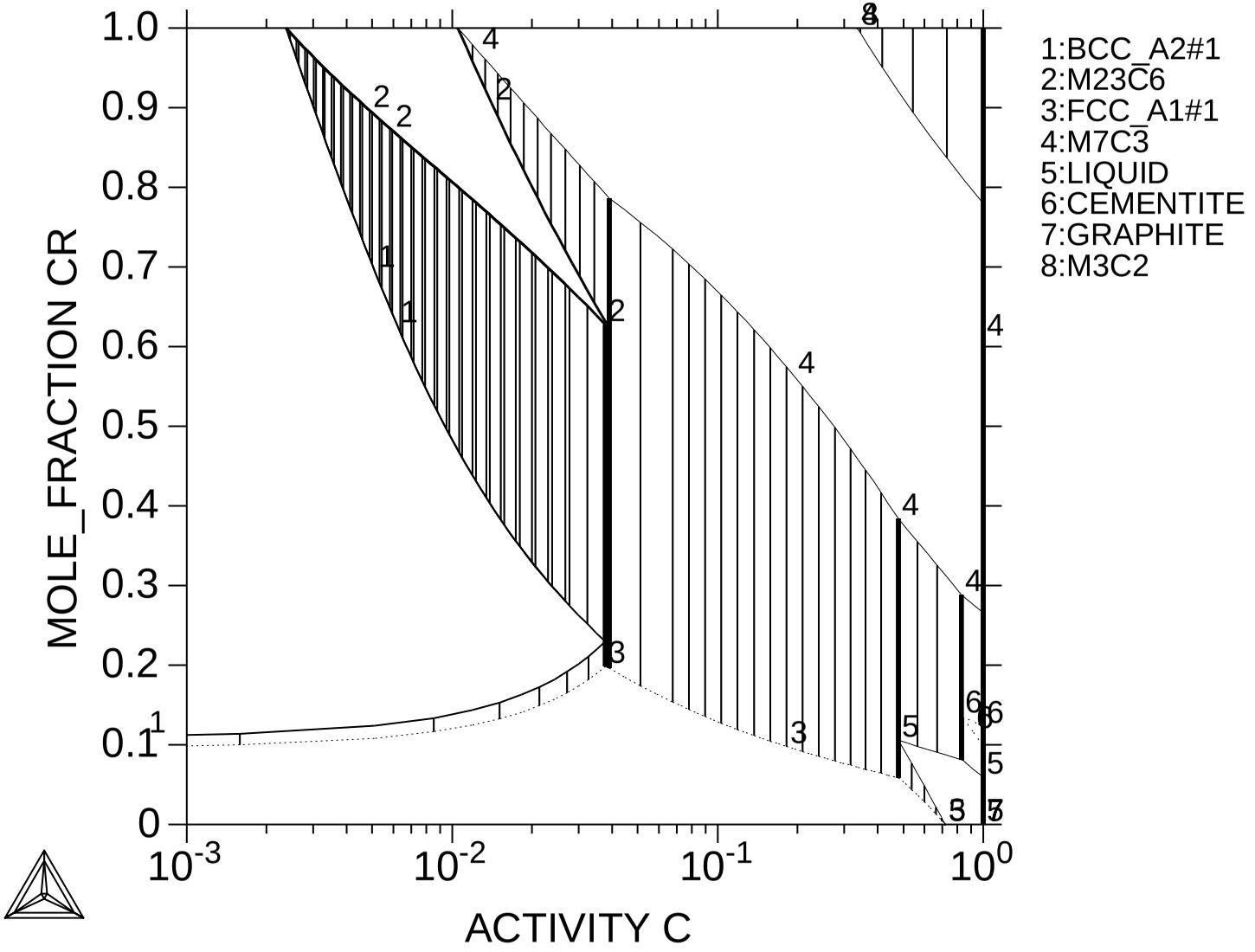
THERMO-CALC (2009.04.29:14.08) :example 3f
DATABASE:PTERN
T=1473.15, P=1E5, N=1;

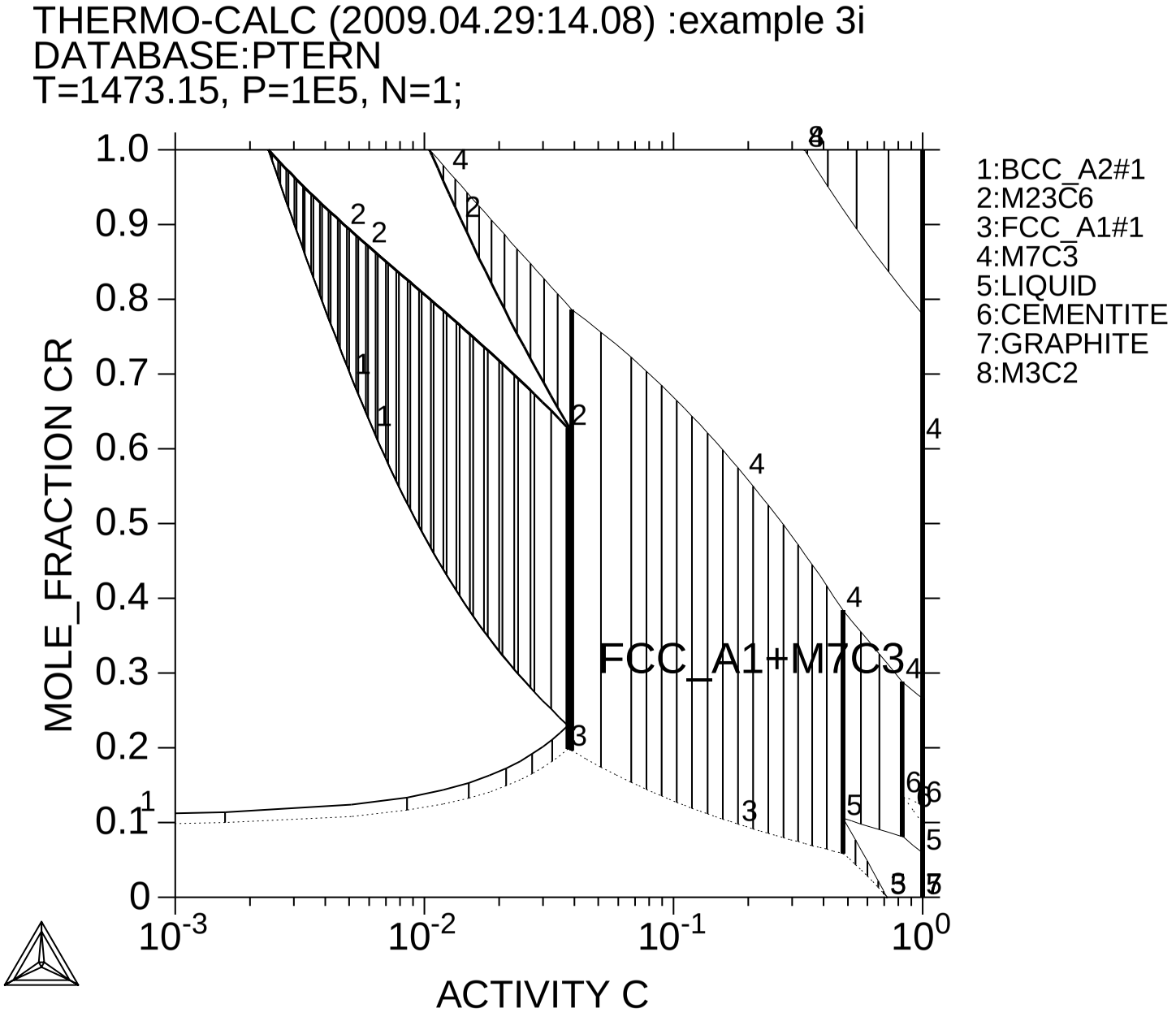


THERMO-CALC (2009.04.29:14.08) :example 3g
DATABASE:PTERN
T=1473.15, P=1E5, N=1;



THERMO-CALC (2009.04.29:14.08) :example 3h
DATABASE:PTERN
T=1473.15, P=1E5, N=1;




THERMO-CALC (2009.04.29:14.08) :example 3i
DATABASE:PTERN
T=1473.15, P=1E5, N=1;
MOLE_FRACTION CR
ACTIVITY C
FCC_A1+M7C3
1:BCC_A2#1
2:M23C6
3:FCC_A1#1
4:M7C3
5:LIQUID
6:CEMENTITE
7:GRAPHITE
8:M3C2

4

Calculation of the Fe-Cr phase diagram (How to handle miscibility gap)

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of the miscibility gap in Fe-Cr
SYS: @@
SYS: @@ From Version R, users do not need to use extra commands to
SYS: @@ handle miscibility map calculations. The Global Minimization
SYS: @@ procedure can find a miscibility gap automatically.
SYS: @@ From Version S, users can use 'MAP' without adding initial
SYS: @@ equilibrium. The new mapping procedure will find all connected
SYS: @@ or non-connected phase boundaries in a phase diagram.
SYS: @@
SYS: set-log ex04,,,
SYS:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw PTERN
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN: def-sys
   ... the command in full is DEFINE_SYSTEM
ELEMENTS: fe cr
 FE                      CR  DEFINED
TDB_PTERN: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 LIQUID:L    :CR FE:
  > This is metallic liquid solution phase, with C species
 FCC_A1      :CR FE:VA:
 BCC_A2      :CR FE:VA:
 HCP_A3      :FE:VA:
 SIGMA       :FE:CR:CR FE:
TDB_PTERN: rej ph /all
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  SIGMA  REJECTED
TDB_PTERN: rest ph liq fcc bcc sigma
   ... the command in full is RESTORE
 LIQUID:L                FCC_A1                  BCC_A2
 SIGMA  RESTORED
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
      (1986); CR-FE'
 -OK-
TDB_PTERN: go p-3
```

```
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 SIGMA                   ENTERED    0.00000000E+00  0.00000000E+00
 FCC_A1                  ENTERED    0.00000000E+00  0.00000000E+00
 BCC_A2                  ENTERED    0.00000000E+00  0.00000000E+00
 LIQUID                  ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 CR ENTERED    FE ENTERED    VA ENTERED
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ There is a miscibility gap in BCC Fe-Cr. Prior to version R, we
POLY_3: @@ must tell the program by the command SPECIAL/SET_MISCIBILITY_GAP.
POLY_3: @@ From version R, the Global Minimization procedure can find the
POLY_3: @@ miscibility gap automatically.
POLY_3: @@ Let us first calculate the low temperature region.
POLY_3: s-c x(cr)=.6 t=700 p=101325 n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          548  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Creating a new composition set BCC_A2#2
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: PTERN

 Conditions:
 X(CR)=0.6, T=700, P=1.01325E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    700.00 K (   426.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.35364E+01
 Total Gibbs energy -2.30650E+04,  Enthalpy  1.31808E+04,  Volume  7.26677E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      6.0000E-01  5.8274E-01 2.3706E-02 -2.1779E+04 SER
 FE                      4.0000E-01  4.1726E-01 1.3646E-02 -2.4994E+04 SER

 BCC_A2#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 6.0119E-01, Mass 3.1438E+01, Volume fraction 6.0387E-01  Mass fractions:
 CR  9.17510E-01  FE  8.24897E-02

 BCC_A2#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 3.9881E-01, Mass 2.2098E+01, Volume fraction 3.9613E-01  Mass fractions:
 FE  8.93536E-01  CR  1.06464E-01
POLY_3:@?
POLY_3: @@ Now make a calculation at a higher temperature
POLY_3: s-c t=900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          548  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: PTERN
```

```
 Conditions:
 X(CR)=0.6, T=900, P=1.01325E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    900.00 K (   626.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.35364E+01
 Total Gibbs energy -3.49339E+04,  Enthalpy  2.36270E+04,  Volume  5.01460E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      6.0000E-01  5.8274E-01 1.2780E-02 -3.2625E+04 SER
 FE                      4.0000E-01  4.1726E-01 5.9093E-03 -3.8397E+04 SER

 SIGMA                       Status ENTERED     Driving force  0.0000E+00
 Moles 6.3242E-01, Mass 3.4078E+01, Volume fraction 4.6246E-01  Mass fractions:
 FE  5.08488E-01  CR  4.91512E-01

 BCC_A2#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 3.6758E-01, Mass 1.9458E+01, Volume fraction 5.3754E-01  Mass fractions:
 CR  7.42505E-01  FE  2.57495E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The Fe-Cr phase diagram has three non-connected two-phase regions.
POLY_3: @@ Prior to version S, it requires three initial equilibria and a special
POLY_3: @@ procedure to help the program to find these regions. From version S,
POLY_3: @@ if the user does not use 'ADD', the new mapping procedure will
POLY_3: @@ automatically find all three non-connected phase regions.
POLY_3: s-a-v 1 x(cr)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  1
Increment /.025/:
POLY_3: s-a-v 2
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/:  t
Min value /0/:  600
Max value /1/:  2200
Increment /40/:
POLY_3: @@ Always a SAVE command before MAP (or STEP) unless
POLY_3: @@ you want to overlay this calculation with an earlier one
POLY_3: save tcex04 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
```

```
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Working hard

 Phase region boundary   1 at:   1.067E-02  1.169E+03
    BCC_A2#1
  ** FCC_A1
 *** Buffer saved on file: tcex04.POLY3
 Calculated           13  equilibria

 Phase region boundary   2 at:   1.067E-02  1.169E+03
    BCC_A2#1
  ** FCC_A1
 Calculated           48  equilibria

 Phase region boundary   3 at:   5.119E-01  6.100E+02
  ** BCC_A2#1
    BCC_A2#2
 Calculated..            2  equilibria
 Terminating at axis limit.

 Phase region boundary   4 at:   5.112E-01  6.000E+02
    BCC_A2#1
  ** BCC_A2#2
 Calculated.            10  equilibria

       :
       :
       :

 Phase region boundary  21 at:   6.876E-01  2.042E+03
    LIQUID
  ** BCC_A2#1
 Calculated           67  equilibria

 Phase region boundary  22 at:   6.876E-01  2.042E+03
    LIQUID
  ** BCC_A2#1
 Calculated           35  equilibria

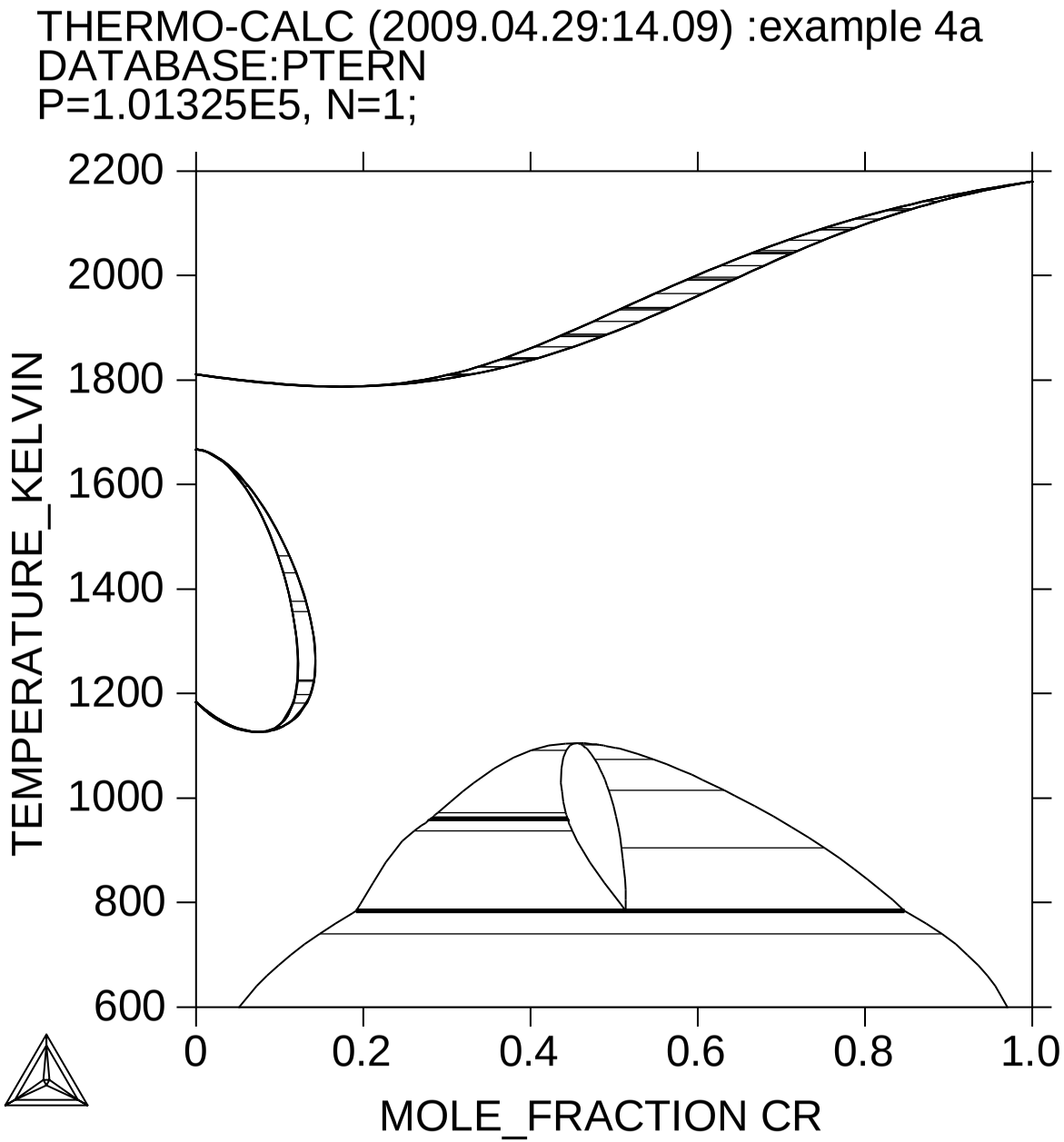
 Phase region boundary  23 at:   9.906E-01  2.178E+03
    LIQUID
  ** BCC_A2#1
 Calculated           92  equilibria

 Phase region boundary  24 at:   9.906E-01  2.178E+03
    LIQUID
  ** BCC_A2#1
 Calculated           15  equilibria
 *** BUFFER SAVED ON FILE: tcex04.POLY3
 CPU time for mapping           4  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,,,,
 *** ERROR  1037 IN GETINT
 *** NO DIGIT
POST:
POST: s-t-s 6
   ... the command in full is SET_TIELINE_STATUS
POST: set_title example 4a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

PLOTFILE : /SCREEN/:
POST:
POST:
POST: **set-inter**
... the command in full is SET_INTERACTIVE_MODE
POST: CPU time 4 seconds


THERMO-CALC (2009.04.29:14.09) :example 4a
DATABASE:PTERN
P=1.01325E5, N=1;
2200
2000
1800
1600
1400
1200
1000
800
600
TEMPERATURE_KELVIN
0
0.2
0.4
0.6
0.8
1.0
MOLE_FRACTION CR

5

Calculation of a vertical section in the Al-Mg-Si system

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of a vertical section from Al to 30% Mg2Si
SYS: @@
SYS: set-log ex05,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw PTERN
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN: def-sys al mg si
   ... the command in full is DEFINE_SYSTEM
 AL                      MG                      SI
   DEFINED
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'N Saunders, COST project (1994); MG-SI'
  'H L Lukas, COST project (1994); AL-SI'
  'H L Lukas, COST project (1994); MG-SI'
  'H L Lukas, COST project (1994); AL-MG-SI'
 -OK-
TDB_PTERN: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1000,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY_3: @@ We shall calculate along a line where the Mg content is twice
POLY_3: @@ that of the Si content, this can be used as a condition.
POLY_3: @@ Note that the whole equation must be given before the equal sign.
POLY_3: @@ It is wrong to write s-c x(mg)=2*x(si).
POLY_3: s-c x(mg)-2*x(si)=0
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1000, P=1E5, N=1, X(MG)-2*X(SI)=0
 DEGREES OF FREEDOM 1
POLY_3: s-c w(si)=0.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         7891  grid points in            0  s
    23 ITS,  CPU TIME USED   0 SECONDS
```

```
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: PTERN

 Conditions:
 T=1000, P=1E5, N=1, X(MG)-2*X(SI)=0, W(SI)=0.1
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.65797E+01
 Total Gibbs energy -4.90158E+04,  Enthalpy  3.04468E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      7.1608E-01  7.2692E-01 4.5195E-03 -4.4893E+04 SER
 MG                      1.8928E-01  1.7308E-01 3.5143E-04 -6.6130E+04 SER
 SI                      9.4640E-02  1.0000E-01 3.9639E-03 -4.5984E+04 SER

 LIQUID                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.6580E+01, Volume fraction 0.0000E+00  Mass fractions:
 AL  7.26918E-01  MG  1.73082E-01  SI  1.00000E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  EXIT                     REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE              SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                     SELECT_EQUILIBRIUM
 BACK                     INFORMATION              SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE       SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS          SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM         SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA  SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS              SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS             SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN          SET_START_VALUE
 DELETE_SYMBOL            MAP                      SHOW_VALUE
 ENTER_SYMBOL             POST                     STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES          TABULATE
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/:  w(si)
Min value /0/:  0
Max value /1/:  .15
Increment /.00375/:  .0025
POLY_3: s-a-v 2
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/:  t
Min value /0/:  500
Max value /1/:  1300
Increment /20/:  10
POLY_3: l-a-v
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(SI)               Min: 0         Max: 0.15      Inc: 2.5E-3
  Axis No 2: T                   Min: 500       Max: 1300      Inc: 10
POLY_3: @?<Hit_return_to_continue>
POLY_3: save tcex05 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
```

```
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24

 Phase region boundary   1 at:   2.500E-03  7.253E+02
     FCC_A1
  ** MG2SI
 *** Buffer saved on file: tcex05.POLY3
 Calculated..           24  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   9.479E-05  5.000E+02
     FCC_A1
  ** MG2SI
 Calculated.           37  equilibria

 Phase region boundary   3 at:   7.819E-03  8.567E+02
  ** LIQUID
     FCC_A1
  ** MG2SI

 Phase region boundary   4 at:   7.819E-03  8.567E+02
     LIQUID
     FCC_A1
  ** MG2SI
 Calculated.           19  equilibria

       :
       :
       :

 Phase region boundary  30 at:   9.917E-02  9.699E+02
     LIQUID
  ** MG2SI
 Calculated.           21  equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   9.917E-02  9.699E+02
     LIQUID
  ** MG2SI
 Calculated..           22  equilibria
```

```
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  32 at:   1.475E-01  1.038E+03
     LIQUID
  ** MG2SI
 Calculated.           41  equilibria
 Terminating at known equilibrium

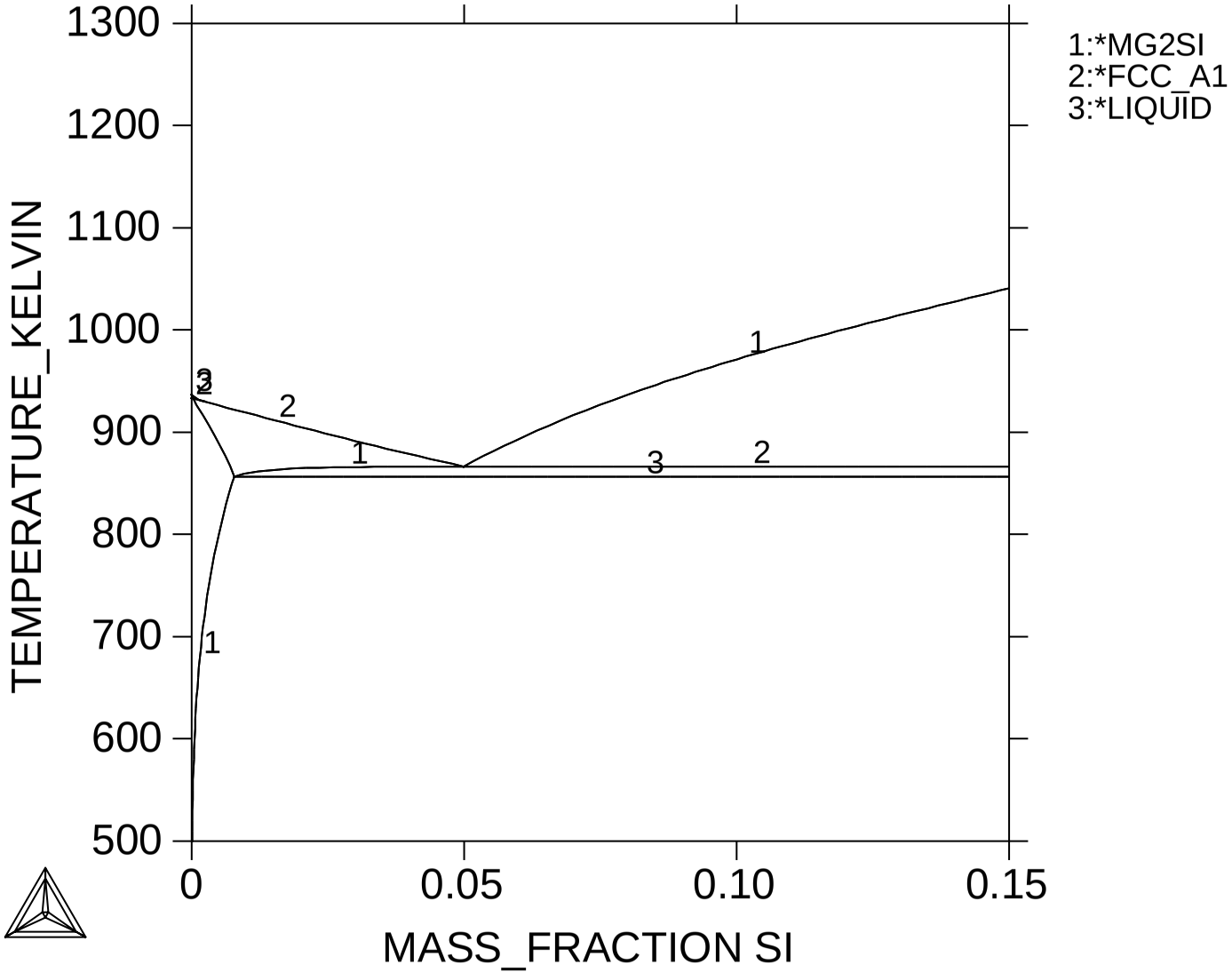
 Phase region boundary  33 at:   1.475E-01  1.038E+03
     LIQUID
  ** MG2SI
 Calculated..           3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: tcex05.POLY3
 CPU time for mapping           5  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

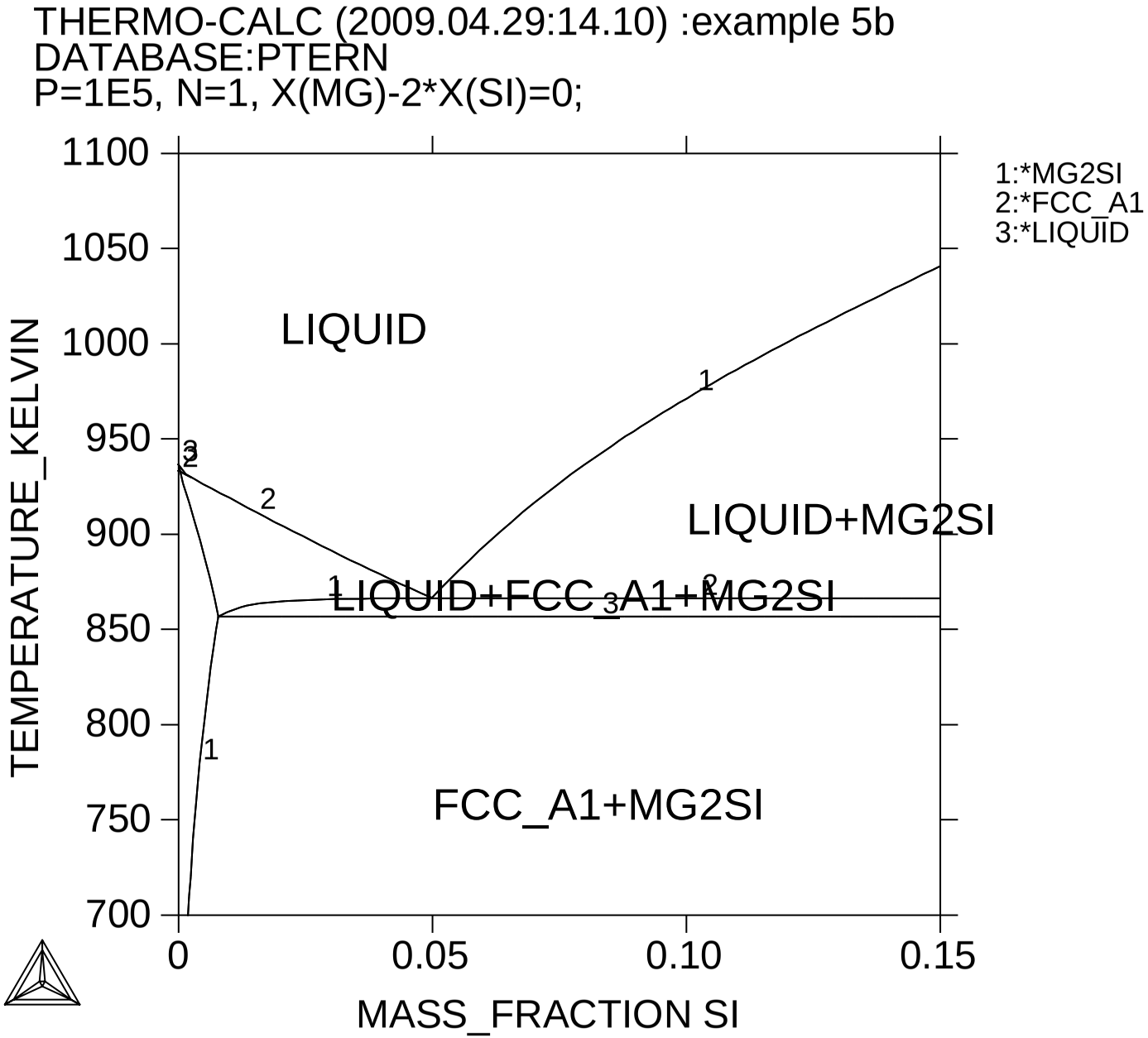
 Setting automatic diagram axis

POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /A/:  b
POST:
POST:
POST: set-title example 5a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-s y n 700 1100
   ... the command in full is SET_SCALING_STATUS
POST: @@ Note that the three-phase region LIQ-FCC-Mg2Si is an area and not
POST: @@ a single line as in a binary system.  This is called a pseudo-binary section
POST: add .05 750
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
 Calculated         7891  grid points in           0  s
 Stable phases are: FCC_A1+MG2SI
Text size: /.3999999762/:
POST: add .02 1000
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
 Calculated         7891  grid points in           0  s
 Stable phases are: LIQUID
Text size: /.3999999762/:
POST: add .1 900
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
 Calculated         7891  grid points in           0  s
 Stable phases are: LIQUID+MG2SI
Text size: /.3999999762/:
POST: add .03 860
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
 Calculated         7891  grid points in           0  s
 Stable phases are: LIQUID+FCC_A1+MG2SI
Text size: /.3999999762/:
POST:
POST: set-title example 5b
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

```
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time            6  seconds
```

THERMO-CALC (2009.04.29:14.10) :example 5a
DATABASE:PTERN
P=1E5, N=1, X(MG)-2*X(SI)=0;




THERMO-CALC (2009.04.29:14.10) :example 5b
DATABASE:PTERN
P=1E5, N=1, X(MG)-2*X(SI)=0;
1100
1050
1000
950
900
850
800
750
700
TEMPERATURE_KELVIN
0
0.05
0.10
0.15
MASS_FRACTION SI
1:*MG2SI
2:*FCC_A1
3:*LIQUID
LIQUID
LIQUID+MG2SI
LIQUID+FCC_A1+MG2SI
FCC_A1+MG2SI
1
2
3

6

Calculation of an isopleth in low alloyed Fe-Mn-Si-Cr-Ni-C steel

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of a multicomponent phase diagram
SYS: @@
SYS: set-log ex06,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ we use the define-material command in POLY and the TCFE steel database
POLY_3: @@ The material contains  1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C
POLY_3: @@ (by weight). These conditions are set by the command and in
POLY_3: @@ addition the temperature. Hidden commands set the pressure to 1 bar
POLY_3: @@ and that iron is "the rest".
POLY_3: @@ After calculating the first equilibrium we calculate a phase diagram
POLY_3: @@ with one axis variable as temperature and the other as the
POLY_3: @@ carbon content
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/:  tcfe6
Major element or alloy: ?
 Major element or alloy

  The material must have a "major" element, usually the element which is
  present in the largest amount. The fraction of this element will not be
  set but be "the rest".

  In some databases there are the "alloys" predefined. An alloy has a
  default major element and have limits of the amounts of the alloying
  elements. If the user stays within there limits the calculation should
  give reasonable results.

Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:  y
1st alloying element: c
Mass (weight) percent /1/:  1
2nd alloying element: si .3
Next alloying element: mn .4
Next alloying element: ni 3.5
Next alloying element: cr 1.5
Next alloying element:
Temperature (C) /1000/:  1000
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
```

```
 This database has following phases for the defined system

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 A1_KAPPA                KAPPA                   FE4N_LP1
 FECN_CHI                SIGMA                   CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   NI3TI                   AL4C3
 FE8SI2C                 SIC

Reject phase(s) /NONE/:  NONE
Restore phase(s): /NONE/:  NONE
 ......................................................

    The following phases are retained in this system:

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 A1_KAPPA                KAPPA                   FE4N_LP1
 FECN_CHI                SIGMA                   CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   NI3TI                   AL4C3
 FE8SI2C                 SIC

 ......................................................

OK? /Y/:  Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J. Grobner, H.L. Lukas and F. Aldinger, Calphad, 20 (1996), 247-254; Si-C
      and Al-Si-C'
                    :
                    :
                    :
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
      (1986); CR-FE-MO'
  'B.-J. Lee, estimated parameter 1999'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'I. Ansara, unpublished work (1991); Cr-Si'
  'A. Bolcavage and U.R. Kattner, J. Phase Equil., 2, (1996); Nb-Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Halite'
 -OK-
Should any phase have a miscibility gap check? /N/:  N
 Using global minimization procedure
 Calculated        24130  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3:
```

```
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=1273.15, W(C)=1E-2, W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2,
    P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1273.15 K (  1000.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.37536E+01
 Total Gibbs energy -6.46529E+04,  Enthalpy  3.76283E+04,  Volume  7.13756E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.4754E-02  1.0000E-02 8.3878E-02 -2.6235E+04 SER
 CR                      1.5507E-02  1.5000E-02 1.2598E-04 -9.5052E+04 SER
 FE                      8.9803E-01  9.3300E-01 2.4771E-03 -6.3521E+04 SER
 MN                      3.9138E-03  4.0000E-03 3.0765E-06 -1.3435E+05 SER
 NI                      3.2056E-02  3.5000E-02 6.1631E-05 -1.0262E+05 SER
 SI                      5.7417E-03  3.0000E-03 6.4662E-09 -1.9961E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3754E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  9.33000E-01  CR  1.50000E-02  MN  4.00000E-03
 NI  3.50000E-02  C   1.00000E-02  SI  3.00000E-03
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Note that values now must be set in fractions and Kelvin!
POLY_3: @@ Sorry about that
POLY_3: s-a-v 1 w(c)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  .01
Increment /2.5E-04/:  1E-4
POLY_3: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  700
Max value /1/:  1300
Increment /15/:
POLY_3: save tcex06 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
```

```
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28

Phase region boundary   1 at:   1.953E-03  7.100E+02
    BCC_A2
    FCC_A1#1
 ** M3C2
    M7C3
*** Buffer saved on file: tcex06.POLY3
Calculated..            3  equilibria
Terminating at axis limit.

Phase region boundary   2 at:   1.810E-03  7.000E+02
    BCC_A2
    FCC_A1#1
 ** M3C2
    M7C3
Calculated.           10  equilibria

Phase region boundary   3 at:   2.222E-03  7.146E+02
    BCC_A2
    FCC_A1#1
 ** GRAPHITE
 ** M3C2
    M7C3

Phase region boundary   4 at:   2.222E-03  7.146E+02
    BCC_A2
    FCC_A1#1
    GRAPHITE
 ** M3C2
    M7C3
Calculated..           80  equilibria
Terminating at axis limit.

      :
      :
      :

Phase region boundary  55 at:   6.633E-03  1.105E+03
 ** CEMENTITE
    FCC_A1#1
Calculated.            7  equilibria
Terminating at known equilibrium

Phase region boundary  56 at:   6.633E-03  1.105E+03
 ** CEMENTITE
    FCC_A1#1
Calculated..           36  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  57 at:   9.900E-03  1.198E+03
 ** CEMENTITE
    FCC_A1#1
Calculated.           39  equilibria
Terminating at known equilibrium
```

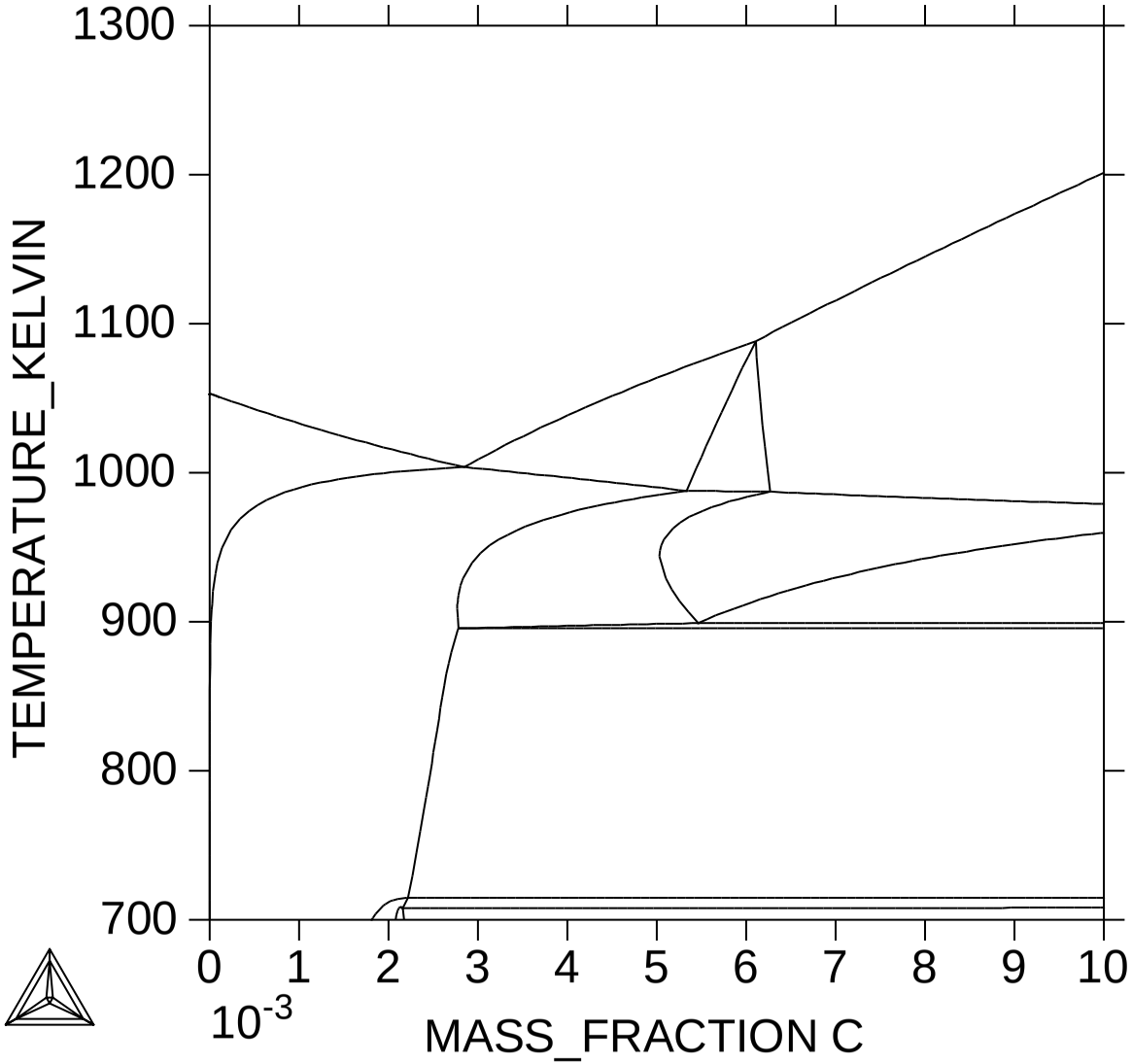
```
 Phase region boundary  58 at:   9.900E-03  1.198E+03
  ** CEMENTITE
     FCC_A1#1
 Calculated..            4  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: tcex06.POLY3
 CPU time for mapping          71  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

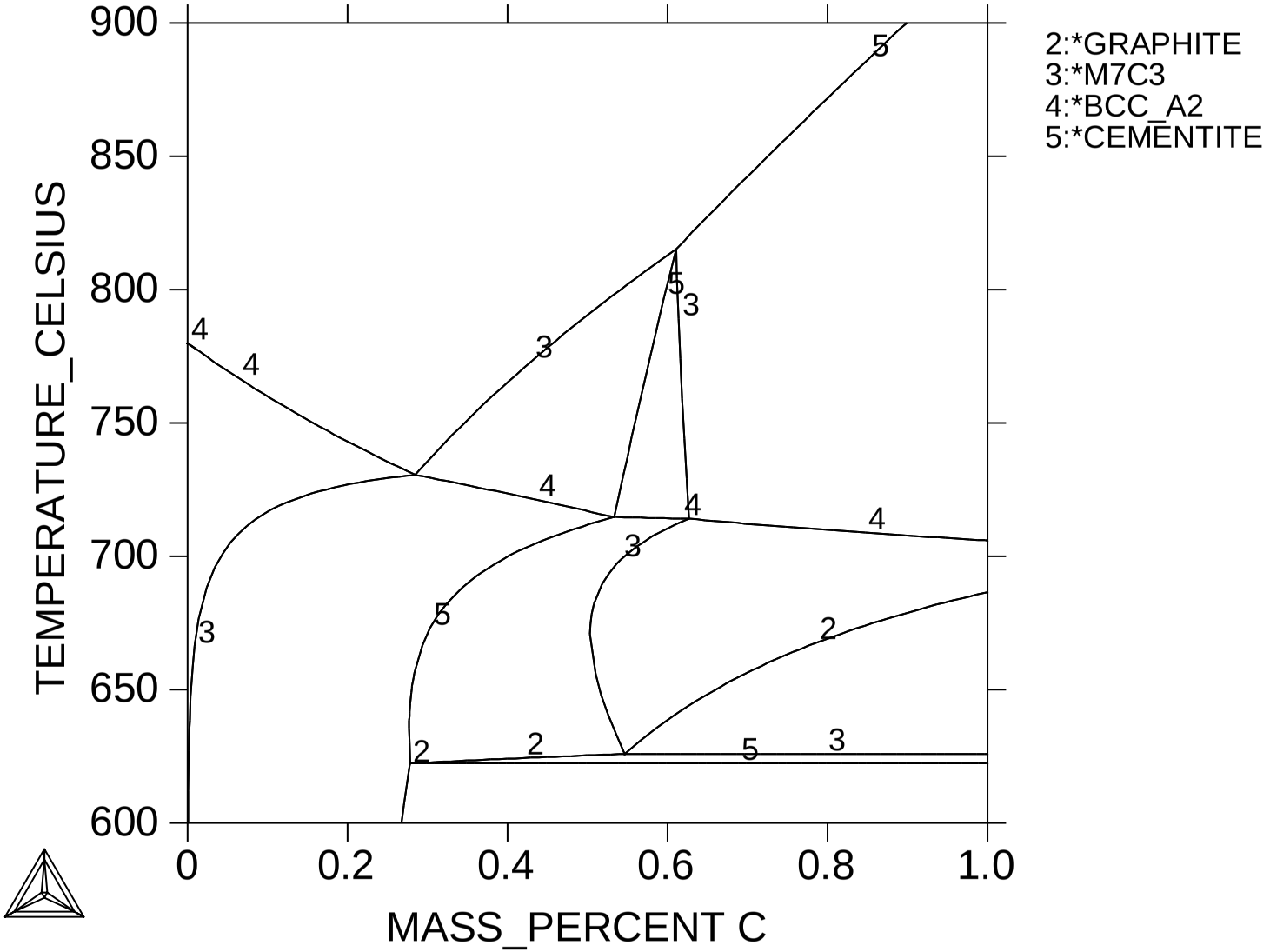
POST:
POST:
POST: set-title example 6a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Use more practical quantities in the plot and
POST: @@ label the curves
POST: s-d-a x w-p c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST:
POST: s-s y n 600 900
   ... the command in full is SET_SCALING_STATUS
POST:
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Determine the phase region at the iron rich side
POST: add .2 850
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated        24130  grid points in           1  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       0 s, total time     1  s
 Stable phases are: FCC_A1
Text size: /.3999999762/:
POST: @@ Knowing that only FCC (or austenite) is stable in that region and
POST: @@ which phase is stable along each line, one can determine the phases
POST: @@ in each region. For example at 0.3 % C and 630 degree C one should
POST: @@ have FCC+BCC+M7C3+CEMENTITE.
POST: @@ Check by adding a label
POST: add .3 630
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated        24130  grid points in           0  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       1 s, total time     1  s
 Stable phases are: BCC_A2+CEMENTIT+FCC_A1+M7C3
Text size: /.3999999762/:
POST: s-lab n
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6c
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

```
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           77  seconds
```

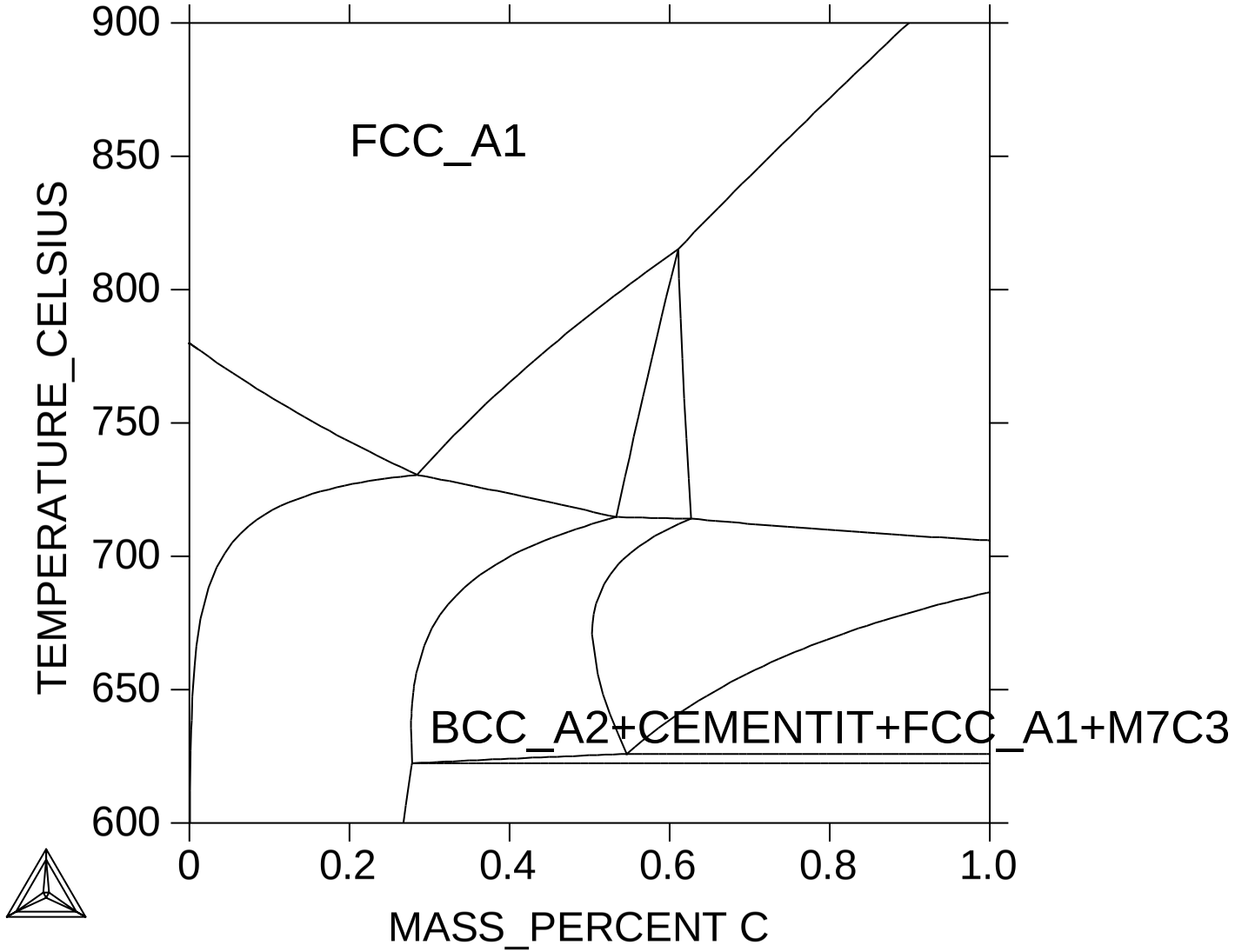
THERMO-CALC (2009.04.15:02.58) :example 6a
DATABASE:TCFE6
W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2, P=1E5, N=1;



THERMO-CALC (2009.04.15:02.58) :example 6b
DATABASE:TCFE6
W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2, P=1E5, N=1;



THERMO-CALC (2009.04.15:02.58) :example 6c
DATABASE:TCFE6
W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2, P=1E5, N=1;



7

Calculation of single equilibria in low alloyed Fe-Mn-Si-Cr-Ni-C steel

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Single equilibrium calculations in a steel
SYS: @@
SYS: @@ There are two common ways to perform a single equilibrium calculation.
SYS: @@ 1) start from scratch: firstly get data from database, then in
SYS: @@    POLY use SET_CONDITION and COMPUTE_EQUILIBRIUM.
SYS: @@ 2) Go directly to POLY, and use DEFINE_MATERIAL.
SYS: @@
SYS: @@ One often wants to know the temperature or composition where one phase
SYS: @@ forms or disappears, COMPUTE_TRANSITION is a useful command. It is the
SYS: @@ same as the CHANGE_STATUS/SET_CONDITION/COMPUTE_EQUILIBRIUM combination.
SYS: @@
SYS: set-log ex07,,
SYS: @@ The alloy composition is 1 wt% Cr, 0.3 wt% Si, 0.3wt% Mn,
SYS: @@ 2.8 wt% Ni and 0.55 wt% C
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/: tcfe6
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .55
2nd alloying element: cr 1
Next alloying element: mn .3 ni 2.8 si .3
Next alloying element:
Temperature (C) /1000/: 600
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED

 This database has following phases for the defined system

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 A1_KAPPA                KAPPA                   FE4N_LP1
 FECN_CHI                SIGMA                   CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   NI3TI                   AL4C3
 FE8SI2C                 SIC
```

```
Reject phase(s) /NONE/:
Restore phase(s): /NONE/:

 ..................................................

    The following phases are retained in this system:

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 A1_KAPPA                KAPPA                   FE4N_LP1
 FECN_CHI                SIGMA                   CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   NI3TI                   AL4C3
 FE8SI2C                 SIC

 ..................................................

OK? /Y/:  Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J. Grobner, H.L. Lukas and F. Aldinger, Calphad, 20 (1996), 247-254; Si-C
      and Al-Si-C'
                    :
                    :
                    :
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
      (1986); CR-FE-MO'
  'B.-J. Lee, estimated parameter 1999'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'I. Ansara, unpublished work (1991); Cr-Si'
  'A. Bolcavage and U.R. Kattner, J. Phase Equil., 2, (1996); Nb-Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Halite'
 -OK-
Should any phase have a miscibility gap check? /N/:  N
 Using global minimization procedure
 Calculated        24130  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3:
POLY_3: @@ The first equilibrium is calculated automatically
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,
    P=1E5, N=1
 DEGREES OF FREEDOM 0
```

```
 Temperature    873.15 K (   600.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.46196E+01
 Total Gibbs energy -3.56732E+04,  Enthalpy  1.79282E+04,  Volume  7.20787E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.5011E-02  5.5000E-03 2.6153E-01 -9.7369E+03 SER
 CR                      1.0505E-02  1.0000E-02 2.4479E-04 -6.0366E+04 SER
 FE                      9.2961E-01  9.5050E-01 8.6789E-03 -3.4461E+04 SER
 MN                      2.9826E-03  3.0000E-03 2.8925E-05 -7.5871E+04 SER
 NI                      2.6058E-02  2.8000E-02 3.4662E-04 -5.7841E+04 SER
 SI                      5.8342E-03  3.0000E-03 2.9885E-11 -1.7593E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.5814E-01, Mass 5.3405E+01, Volume fraction 9.6729E-01  Mass fractions:
 FE  9.63504E-01  SI  3.06820E-03  MN  2.28601E-03
 NI  2.85952E-02  CR  2.52703E-03  C   1.97123E-05

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 2.4194E-02, Mass 1.0019E+00, Volume fraction 1.9532E-02  Mass fractions:
 FE  4.58650E-01  C   8.70086E-02  NI  2.20485E-03
 CR  4.10444E-01  MN  4.16928E-02  SI  0.00000E+00

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.7665E-02, Mass 2.1218E-01, Volume fraction 1.3181E-02  Mass fractions:
 C   1.00000E+00  NI  0.00000E+00  FE  0.00000E+00
 SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
POLY_3: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  EXIT                      REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE               SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                      SELECT_EQUILIBRIUM
 BACK                     INFORMATION               SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE        SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS           SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM          SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA   SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS               SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS              SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM  SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN           SET_START_VALUE
 DELETE_SYMBOL            MAP                       SHOW_VALUE
 ENTER_SYMBOL             POST                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES           TABULATE
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Increase Cr until all Graphite disappears. Calculate this
POLY_3: @@ directly using the COMPUTE-TRANSITION command.  You
POLY_3: @@ must release the Cr content of course
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: grap
 You must release one of these conditions
 T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,
 P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/:  w(cr)
 Testing POLY result by global minimization procedure
 Using already calculated grid
To form GRAP the condition is set to W(CR)=.0293768365616
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=873.15, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
    W(SI)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    873.15 K (   600.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45430E+01
 Total Gibbs energy -3.61950E+04,  Enthalpy  1.77828E+04,  Volume  7.15532E-06
```

```
 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.4976E-02  5.5000E-03 2.6153E-01 -9.7369E+03 SER
 CR                      3.0816E-02  2.9377E-02 2.5353E-04 -6.0112E+04 SER
 FE                      9.0938E-01  9.3112E-01 8.6730E-03 -3.4466E+04 SER
 MN                      2.9784E-03  3.0000E-03 1.8254E-05 -7.9213E+04 SER
 NI                      2.6022E-02  2.8000E-02 3.6127E-04 -5.7540E+04 SER
 SI                      5.8260E-03  3.0000E-03 3.1190E-11 -1.7562E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.1702E-01, Mass 5.1110E+01, Volume fraction 9.3250E-01  Mass fractions:
 FE  9.62968E-01  SI  3.20151E-03  MN  1.45355E-03
 NI  2.97317E-02  CR  2.62575E-03  C   1.94050E-05

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 8.2978E-02, Mass 3.4330E+00, Volume fraction 6.7498E-02  Mass fractions:
 FE  4.57021E-01  C   8.70942E-02  NI  2.21880E-03
 CR  4.27642E-01  MN  2.60233E-02  SI  0.00000E+00

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 C   1.00000E+00  NI  0.00000E+00  FE  0.00000E+00
 SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Graphite disappears when we have this chromium content 3.15 w/o
POLY_3: @@ The amount of Cr can be obtain directly with a show command
POLY_3: show w(cr)
   ... the command in full is SHOW_VALUE
 W(CR)=2.9376837E-2
POLY_3: @@ This is automatically set as new condition by the C-T command
POLY_3: @@ and the amount of graphite is zero.
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FCC_A1#1                ENTERED    3.19064452E+00  0.00000000E+00
 M7C3                    ENTERED    0.00000000E+00  8.29780469E-02
 GRAPHITE                ENTERED    0.00000000E+00  0.00000000E+00
 BCC_A2                  ENTERED    0.00000000E+00  9.17021937E-01
 CEMENTITE               ENTERED   -1.68484607E-02  0.00000000E+00
 FCC_A1#2                ENTERED   -1.78577528E-02  0.00000000E+00
 M23C6                   ENTERED   -9.18779718E-02  0.00000000E+00
 KAPPA                   ENTERED   -1.72879062E-01  0.00000000E+00
 M3C2                    ENTERED   -2.52230463E-01  0.00000000E+00
 HCP_A3#2                ENTERED   -2.61784169E-01  0.00000000E+00
 HCP_A3#1                ENTERED   -2.61784169E-01  0.00000000E+00
 FECN_CHI                ENTERED   -3.86725147E-01  0.00000000E+00
 M5C2                    ENTERED   -5.59729274E-01  0.00000000E+00
 LIQUID                  ENTERED   -6.75368073E-01  0.00000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN -7.16680812E-01
 SIGMA CHI_A12 DIAMOND_FCC_A4 FE4N_LP1 LAVES_PHASE_C14 KSI_CARBIDE FE8SI2C
 M3SI NI3TI FE2SI NBNI3 CR3SI M5SI3 MSI SIC AL4C3
POLY_3: @@ Now determine the maximum temperature with no Austenite (FCC_A1),
POLY_3: @@ i.e. A1 temperature.
POLY_3: @@ We use again the new command COMPUTE-TRANSITION
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: fcc
 You must release one of these conditions
 T=873.15, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
 W(SI)=3E-3, P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/:  t
 Testing POLY result by global minimization procedure
 Calculated        24130  grid points in           0  s
To form FCC the condition is set to T=915.22062277
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
    W(SI)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY_3: @@ This command does the same as the change-status/set-cond/compute-equil,
POLY_3: @@ Notice that the temperature is set back as condition with the new value.
```

```
POLY_3: @@ If we want temperatures in Celsius we can enter a function.
POLY_3: ent fun tc=t-273;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh tc
   ... the command in full is SHOW_VALUE
 TC=642.22062
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
    W(SI)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    915.22 K (   642.07 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45430E+01
 Total Gibbs energy -3.88407E+04,  Enthalpy  1.96981E+04,  Volume  7.16989E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.4976E-02  5.5000E-03 2.1560E-01 -1.1676E+04 SER
 CR                      3.0816E-02  2.9377E-02 2.6256E-04 -6.2742E+04 SER
 FE                      9.0938E-01  9.3112E-01 7.6560E-03 -3.7076E+04 SER
 MN                      2.9784E-03  3.0000E-03 1.5918E-05 -8.4071E+04 SER
 NI                      2.6022E-02  2.8000E-02 2.9594E-04 -6.1831E+04 SER
 SI                      5.8260E-03  3.0000E-03 6.4895E-11 -1.7851E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.1724E-01, Mass 5.1116E+01, Volume fraction 9.3276E-01  Mass fractions:
 FE  9.61872E-01  CR  3.48152E-03  MN  1.68770E-03
 NI  2.97230E-02  SI  3.20115E-03  C   3.45703E-05

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 8.2763E-02, Mass 3.4273E+00, Volume fraction 6.7240E-02  Mass fractions:
 FE  4.72522E-01  C   8.70137E-02  NI  2.30172E-03
 CR  4.15590E-01  MN  2.25722E-02  SI  0.00000E+00

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.68031E-01  MN  1.44441E-02  SI  4.18888E-03
 NI  1.05328E-01  CR  5.51928E-03  C   2.48820E-03
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:  cps
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 NI                      ENTERED   SER
 SI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 M7C3                    ENTERED    0.00000000E+00  8.27628828E-02
 FCC_A1#2                ENTERED    0.00000000E+00  0.00000000E+00
 FCC_A1#1                ENTERED    0.00000000E+00  0.00000000E+00
 BCC_A2                  ENTERED    0.00000000E+00  9.17237125E-01
 CEMENTITE               ENTERED   -6.42271641E-03  0.00000000E+00
 M23C6                   ENTERED   -7.33499055E-02  0.00000000E+00
 GRAPHITE                ENTERED   -1.32754768E-01  0.00000000E+00
 KAPPA                   ENTERED   -1.37053121E-01  0.00000000E+00
 HCP_A3#2                ENTERED   -2.51381355E-01  0.00000000E+00
 HCP_A3#1                ENTERED   -2.51381355E-01  0.00000000E+00
 M3C2                    ENTERED   -3.04188617E-01  0.00000000E+00
 FECN_CHI                ENTERED   -3.82641419E-01  0.00000000E+00
 M5C2                    ENTERED   -5.42047478E-01  0.00000000E+00
 LIQUID                  ENTERED   -5.84129847E-01  0.00000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN -6.55881939E-01
```

```
 SIGMA CHI_A12 FE4N_LP1 LAVES_PHASE_C14 DIAMOND_FCC_A4 KSI_CARBIDE FE8SI2C
 M3SI FE2SI NI3TI NBNI3 M5SI3 CR3SI MSI SIC AL4C3
 *** STATUS FOR ALL SPECIES
 C  ENTERED    FE ENTERED    NI ENTERED    VA ENTERED
 CR ENTERED    MN ENTERED    SI ENTERED
POLY_3: @@ Now determine maximum temperature where no Ferrite (BCC_A2) exists
POLY_3: @@ Use
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc
You want to find when the current major phase is formed, please give
New major phase: fcc
 You must release one of these conditions
 T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
 W(SI)=3E-3, P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/:  t
 Testing POLY result by global minimization procedure
 Calculated        24130  grid points in           1  s
To form BCC the condition is set to T=1012.45181313
POLY_3:
POLY_3: show tc
   ... the command in full is SHOW_VALUE
 TC=739.45181
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Check how this varies with the carbon content
POLY_3: ch-st phase fcc
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:  ent
Start value, number of moles /0/:  1
POLY_3: ch-st phase bcc
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:  fix
Number of moles /0/:  0
POLY_3:
POLY_3: s-c t=none
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated        24130  grid points in           0  s
     7 ITS,  CPU TIME USED   1 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3, P=1E5,
    N=1
 FIXED PHASES
 BCC_A2=0
 DEGREES OF FREEDOM 0

 Temperature   1012.45 K (   739.30 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45430E+01
 Total Gibbs energy -4.54060E+04,  Enthalpy  2.77487E+04,  Volume  7.08402E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.4976E-02  5.5000E-03 7.8817E-02 -2.1387E+04 SER
 CR                      3.0816E-02  2.9377E-02 4.6417E-04 -6.4611E+04 SER
 FE                      9.0938E-01  9.3112E-01 5.7861E-03 -4.3372E+04 SER
 MN                      2.9784E-03  3.0000E-03 4.5168E-06 -1.0361E+05 SER
 NI                      2.6022E-02  2.8000E-02 8.0605E-05 -7.9348E+04 SER
 SI                      5.8260E-03  3.0000E-03 3.6734E-10 -1.8288E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.6176E-01, Mass 5.2968E+01, Volume fraction 9.6838E-01  Mass fractions:
 FE  9.46531E-01  CR  1.55549E-02  C   3.06184E-03
 NI  2.88106E-02  SI  3.08922E-03  MN  2.95285E-03

 M7C3                        Status ENTERED     Driving force  0.0000E+00
```

```
 Moles 3.8245E-02, Mass 1.5752E+00, Volume fraction 3.1623E-02  Mass fractions:
 CR  4.94158E-01  C   8.74860E-02  NI  7.42624E-04
 FE  4.13028E-01  MN  4.58537E-03  SI  0.00000E+00

 BCC_A2                      Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.71740E-01  CR  1.04725E-02  MN  8.83251E-04
 NI  1.30178E-02  SI  3.81249E-03  C   7.40352E-05
POLY_3: show tc
   ... the command in full is SHOW_VALUE
 TC=739.45181
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: s-a-v 1 w(c) 0 .08 0.001,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex07 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value   0.550000E-02
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from   0.550000E-02 for:
     BCC_A2
     FCC_A1#1
     M7C3
 Global check of adding phase at  8.31547E-03
 Calculated     5 equilibria

 Phase Region from   0.831547E-02 for:
     BCC_A2
     CEMENTITE
     FCC_A1#1
     M7C3
 Global check of removing phase at  1.15396E-02
 Calculated     7 equilibria

 Phase Region from   0.115396E-01 for:
     BCC_A2
     CEMENTITE
     FCC_A1#1
 Global test at  1.95000E-02 .... OK
 Global check of adding phase at  2.30282E-02
 Calculated    14 equilibria

 Phase Region from   0.230282E-01 for:
     BCC_A2
     CEMENTITE
     FCC_A1#1
     GRAPHITE
 Global test at  3.05000E-02 .... OK
 Global test at  4.05000E-02 .... OK
 Global test at  5.05000E-02 .... OK
 Global test at  6.05000E-02 .... OK
 Global test at  7.05000E-02 .... OK
 Global test at  8.00000E-02 .... OK
 Terminating at   0.800000E-01
 Calculated    61 equilibria

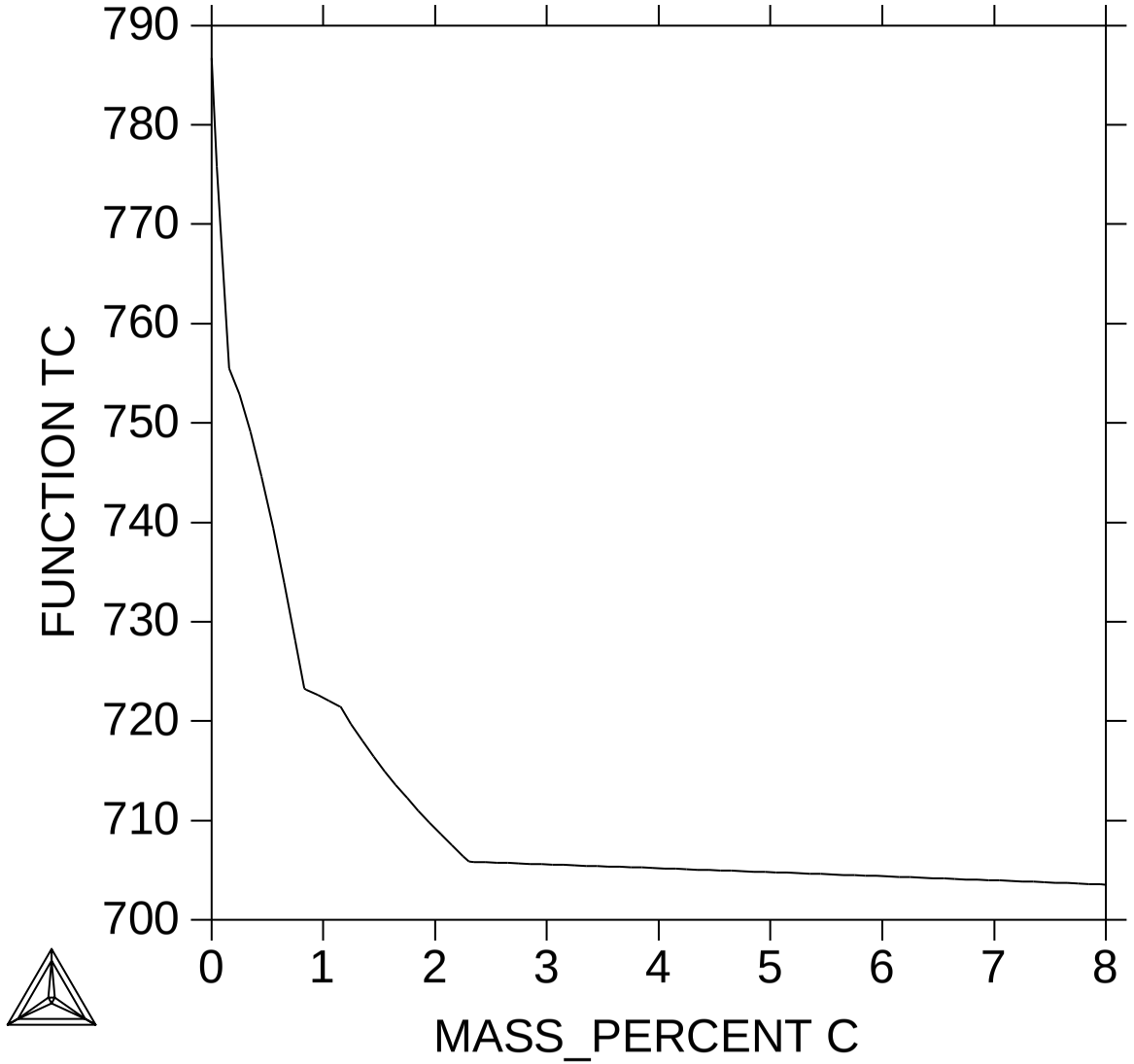
 Phase Region from   0.550000E-02 for:
     BCC_A2
     FCC_A1#1
     M7C3
 Global check of removing phase at  1.56897E-03
 Calculated     6 equilibria

 Phase Region from   0.156897E-02 for:
     BCC_A2
     FCC_A1#1
```

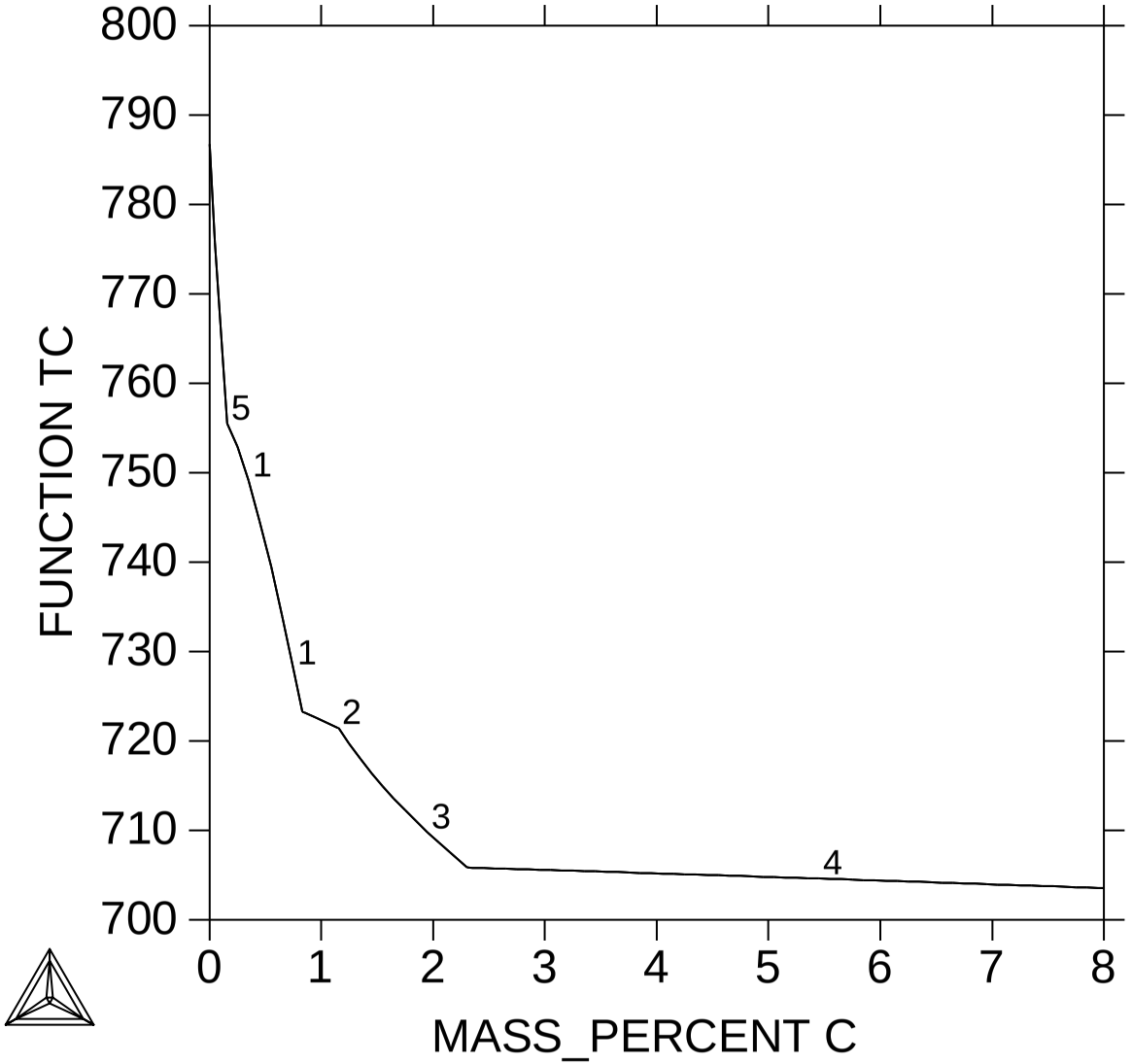
```
 Global test at  9.99743E-16 .... OK
 Terminating at   0.215894E-12
 Calculated     5 equilibria
 *** Buffer saved on file: tcex07.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-d-a x w-p c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y tc
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 7a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-s y n 700 800
   ... the command in full is SET_SCALING_STATUS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 7b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time          14  seconds
```

THERMO-CALC (2009.04.15:02.59) :example 7a
DATABASE:TCFE6
W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3, P=1E5, N=1. FIXED PHASES



THERMO-CALC (2009.04.15:02.59) :example 7b
DATABASE:TCFE6
W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3, P=1E5, N=1. FIXED PHASES



1: F+ BCC_A2 FCC_A1#1 M7C3
2: F+ BCC_A2 CEMENTITE FCC_A1#1 M7C3
3: F+ BCC_A2 CEMENTITE FCC_A1#1
4: F+ BCC_A2 CEMENTITE FCC_A1#1 GRAPHITE
5: F+ BCC_A2 FCC_A1#1

8

Calculation of property diagrams for a high speed steel

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of a property diagram for a high speed steel
SYS: @@ i.e. phase fraction plots, activity vs temperature etc
SYS: @@
SYS: set-log ex08,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: def-dia
   ... the command in full is DEFINE_DIAGRAM
 For binary or ternary diagrams you may prefer the special modules

 You must specify a value for all compositions and the temperature even
 if you want to use it as axis.
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/: tcfe6
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .9 cr 4 mn .3 si .3 w 8 mo 5 v 2
Next alloying element:
Temperature (C) /1000/: 1000
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 W  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MO  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 V  DEFINED

 This database has following phases for the defined system

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 A1_KAPPA                KAPPA                   Z_PHASE
 FE4N_LP1                FECN_CHI                SIGMA
 MU_PHASE                P_PHASE                 R_PHASE
 CHI_A12                 LAVES_PHASE_C14         M3SI
 CR3SI                   FE2SI                   MSI
 M5SI3                   AL4C3                   FE8SI2C
 SIC

Reject phase(s) /NONE/: NONE
```

```
Restore phase(s): /NONE/:  NONE
 ....................................................

    The following phases are retained in this system:

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 A1_KAPPA                KAPPA                   Z_PHASE
 FE4N_LP1                FECN_CHI                SIGMA
 MU_PHASE                P_PHASE                 R_PHASE
 CHI_A12                 LAVES_PHASE_C14         M3SI
 CR3SI                   FE2SI                   MSI
 M5SI3                   AL4C3                   FE8SI2C
 SIC

 ....................................................

OK? /Y/:  Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'J-O. Andersson, Calphad, 12 (1988), 1-8; TRITA 0317 (1986); C-MO'
  'J. Grobner, H.L. Lukas and F. Aldinger, Calphad, 20 (1996), 247-254; Si-C
      and Al-Si-C'
                    :
                    :
                    :
  'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
  'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
  'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'COST2 database 1997'
  'I. Ansara, unpublished work (1991); Cr-Si'
 -OK-
Should any phase have a miscibility gap check? /N/:  N
 Using global minimization procedure
 Calculated        28137  grid points in            1  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     1  s
 You must now set an independent axis for your diagram
 as one of the following conditions:
 Condition  1 is temperature (Celsius)
 Condition  2 is mass percent of C
 Condition  3 is mass percent of CR
 Condition  4 is mass percent of MN
 Condition  5 is mass percent of SI
 Condition  6 is mass percent of W
 Condition  7 is mass percent of MO
 Condition  8 is mass percent of V
Give the number of the condition to vary /1/:  1
Minimum value (C) /800/:  600
Maximum value (C) /1800/:  1600
 The second axis can be another of the conditions above and you will then
```

```
 calculate a phase diagram.
 Or you may want to plot how some other quantities depend on the selected
 condition and you will then calculate a  "property" diagram.

 In addition to the conditions above you may use these selected
 dependent quantities on the vertical axis:
 Dependent  9 is mass fraction of all phases
 Dependent 10 is composition of a phase
 Dependent 11 is the fraction of a component in all phases
 (In the post processor you may select many other quantities)
Give the number of the quantity on second axis /9/: 9 tcex08 y
 No initial equilibrium, using default
 Step will start from axis value    1273.15
 Global calculation of initial equilibrium ....OK

 Phase Region from    1273.15     for:
     FCC_A1#1
     FCC_A1#2
     M6C
 Global test at  1.35315E+03 .... OK
 Global test at  1.45315E+03 .... OK
 Global check of adding phase at  1.52350E+03
 Calculated    28 equilibria

 Phase Region from    1523.50     for:
     LIQUID
     FCC_A1#1
     FCC_A1#2
     M6C
 Global check of removing phase at  1.52405E+03
 Calculated     3 equilibria

 Phase Region from    1524.05     for:
     LIQUID
     FCC_A1#1
     M6C
 Global check of adding phase at  1.57026E+03
 Calculated     7 equilibria

 Phase Region from    1570.26     for:
     LIQUID
     BCC_A2
     FCC_A1#1
     M6C
 Global check of removing phase at  1.57695E+03
 Calculated     4 equilibria

       :
       :
       :

 Phase Region from    1273.15     for:
     FCC_A1#1
     FCC_A1#2
     M6C
 Global test at  1.19315E+03 .... OK
 Global check of adding phase at  1.13904E+03
 Calculated    16 equilibria

 Phase Region from    1139.04     for:
     FCC_A1#1
     FCC_A1#2
     M23C6
     M6C
 Global check of adding phase at  1.11371E+03
 Calculated     5 equilibria

 Phase Region from    1113.71     for:
     BCC_A2
     FCC_A1#1
     FCC_A1#2
     M23C6
     M6C
 Global check of removing phase at  1.09623E+03
```

```
 Calculated     5 equilibria

 Phase Region from    1096.23     for:
     BCC_A2
     FCC_A1#2
     M23C6
     M6C
 Global test at  1.02315E+03 .... OK
 Global test at  9.23150E+02 .... OK
 Terminating at    873.150
 Calculated    26 equilibria
 *** Buffer saved on file: tcex08.POLY3

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is REINITIATE_PLOT_SETTINGS

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

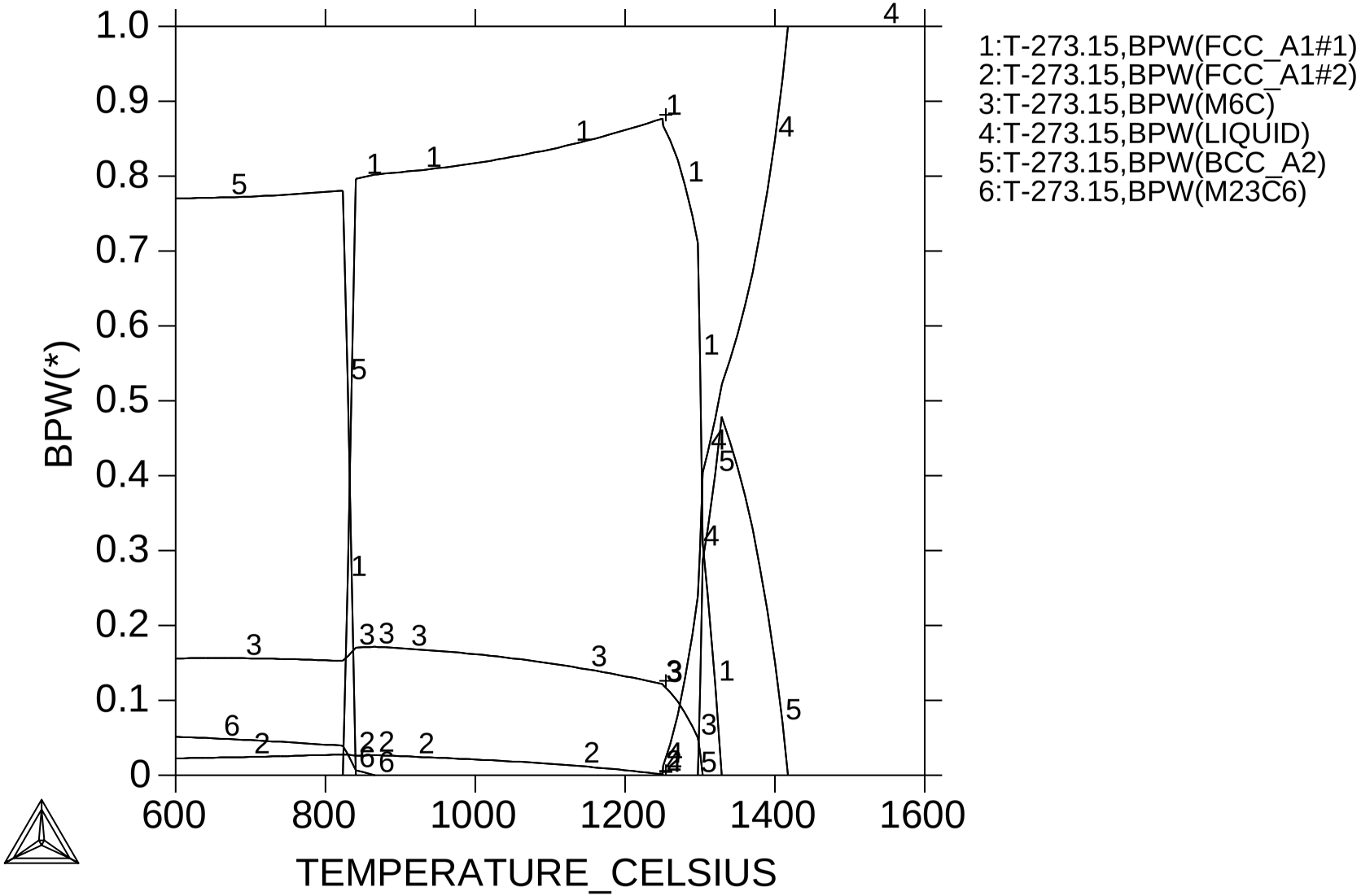
 Setting automatic diagram axis

   ... the command in full is SET_AUTOMATIC_DIAGRAM_A

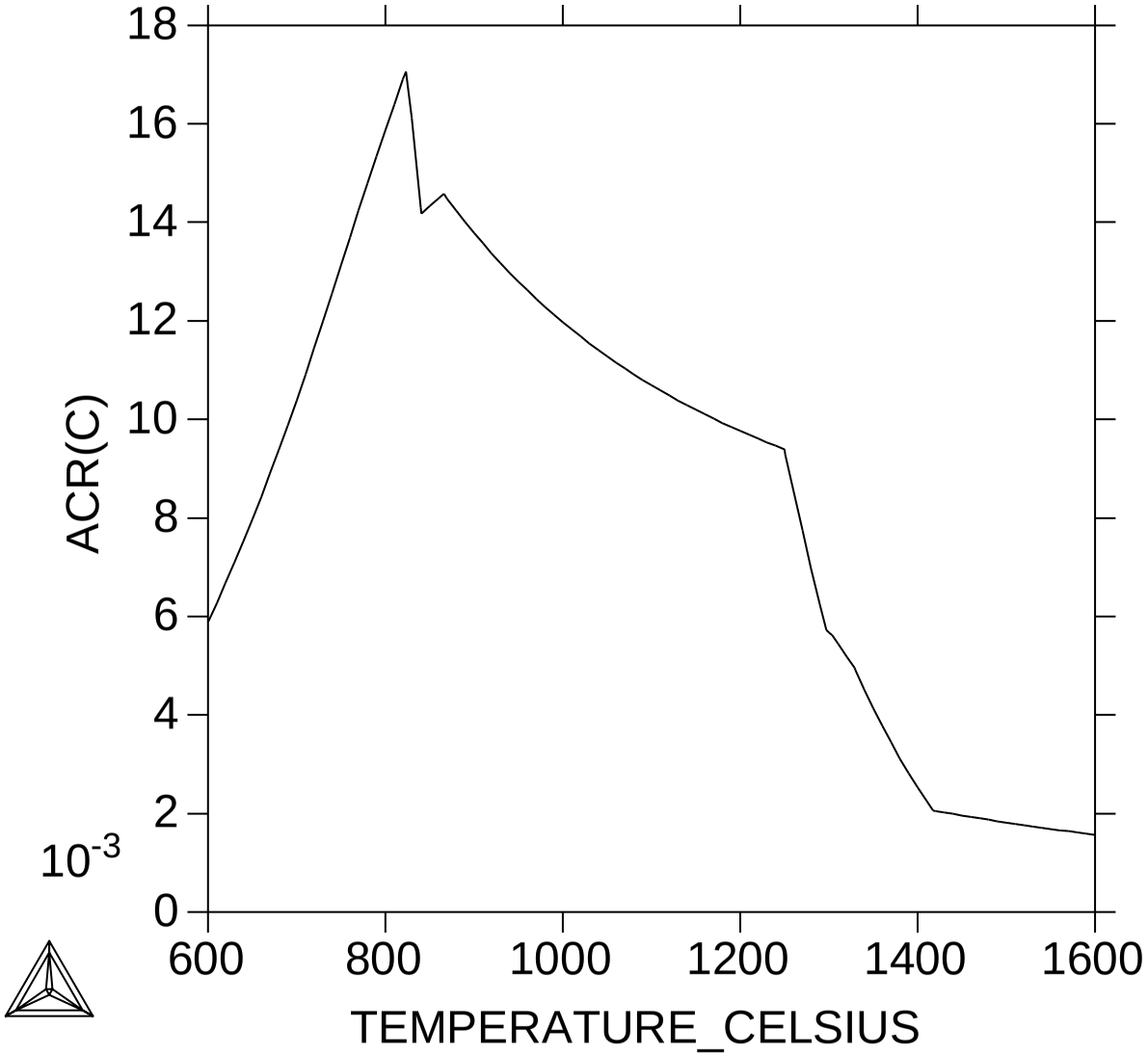
 Setting automatic diagram axis

   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-title example 8a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-d-a y acr(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set_lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N:  n
POST: set-title example 8b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Plot how the composition of the austenite (called fcc) varies
POST: @@ Note this is plotted also where the austenite is not stable!
POST: s-d-a y w(fcc,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set_lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 8c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Plot the fraction of Cr in all phases
POST: s-d-a y w(*,cr)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 8d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time          26  seconds
```

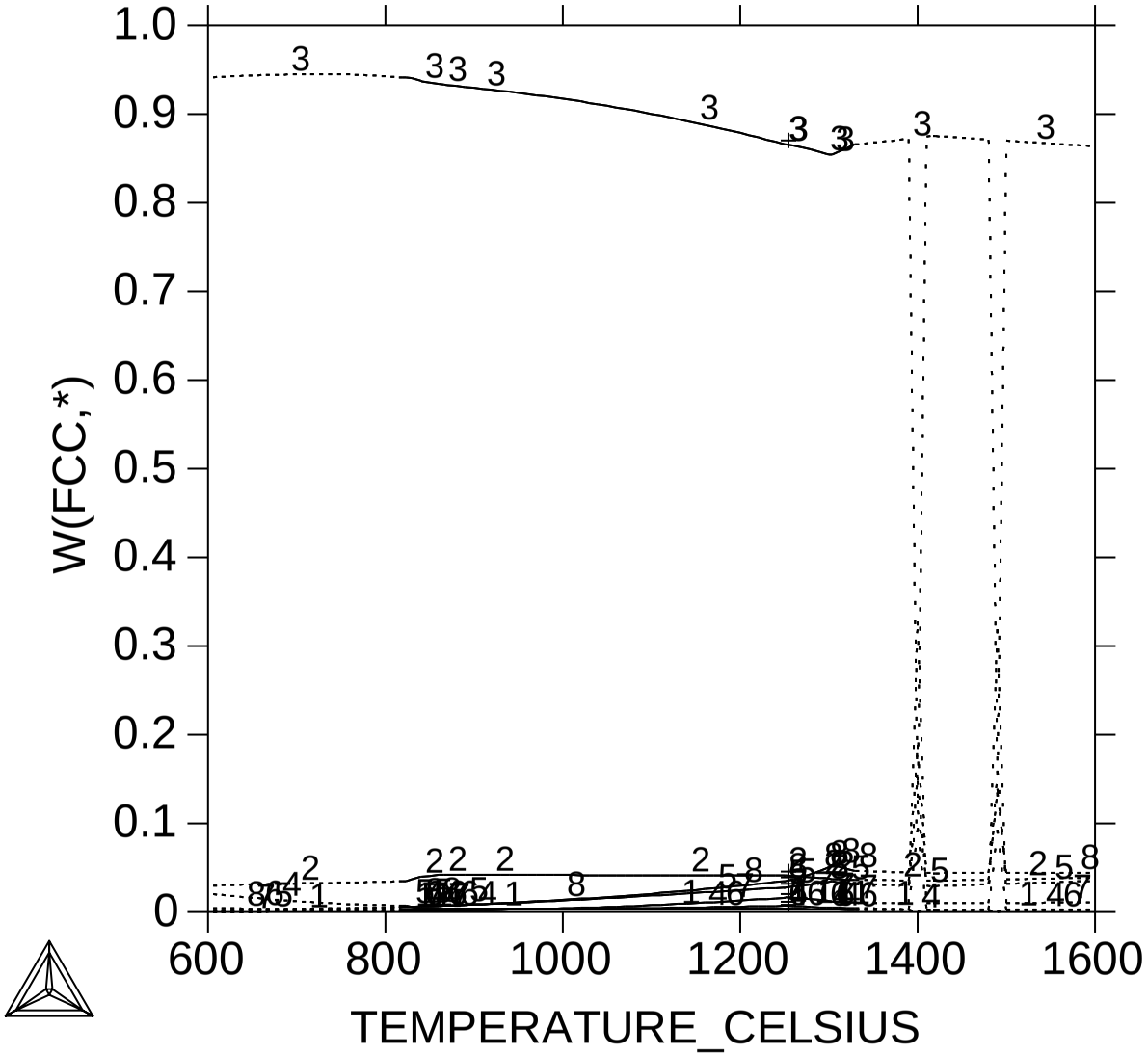
THERMO-CALC (2009.04.15:02.59) :example 8a
DATABASE:TCFE6
W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2,
W(V)=2E-2, P=1E5, N=1.;



THERMO-CALC (2009.04.15:02.59) :example 8b
DATABASE:TCFE6
W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2,
W(V)=2E-2, P=1E5, N=1.;

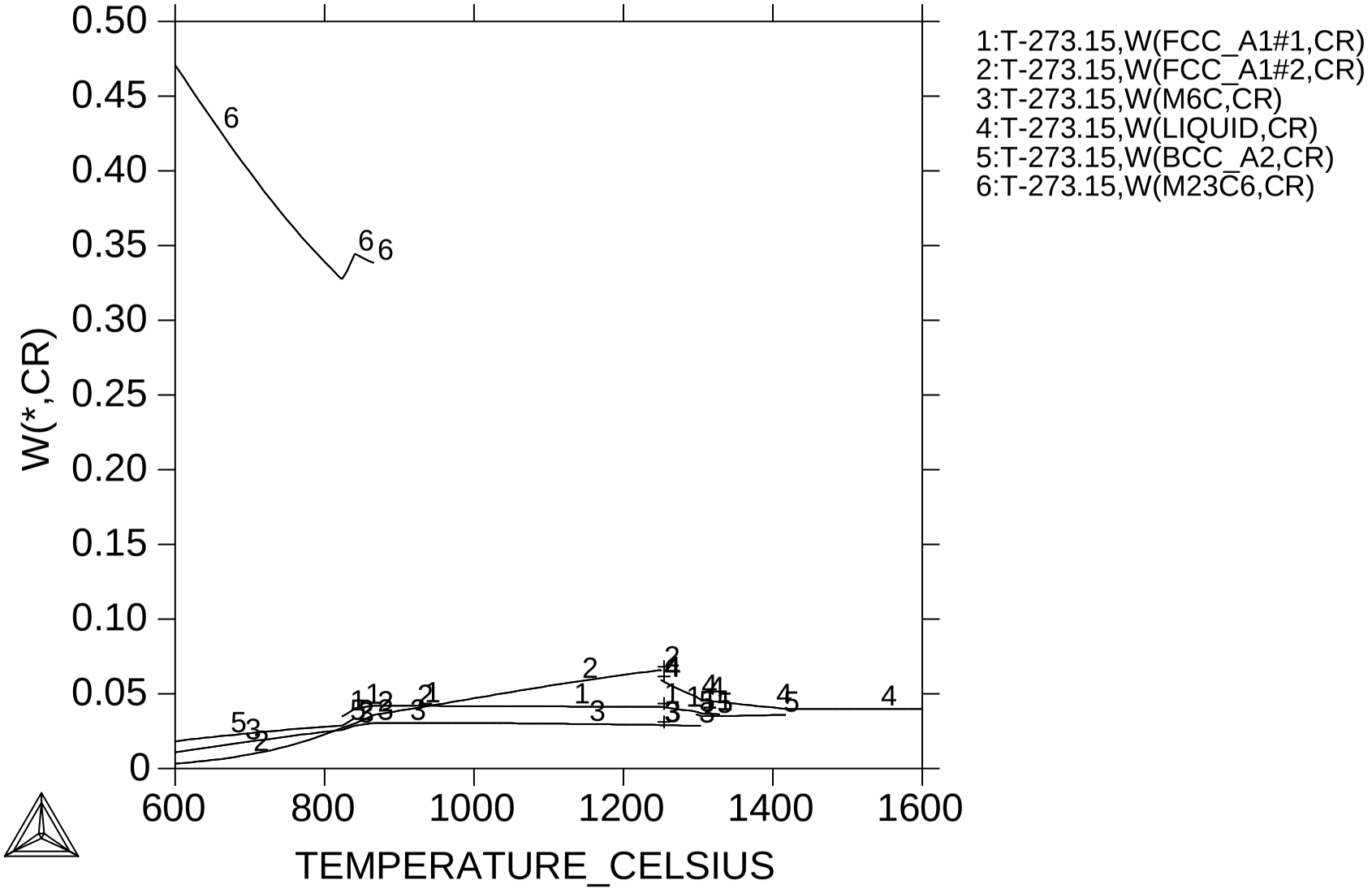


THERMO-CALC (2009.04.15:02.59) :example 8c
DATABASE:TCFE6
W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2,
W(V)=2E-2, P=1E5, N=1.;



1:T-273.15,W(FCC_A1#1,C)
2:T-273.15,W(FCC_A1#1,CR)
3:T-273.15,W(FCC_A1#1,FE)
4:T-273.15,W(FCC_A1#1,MN)
5:T-273.15,W(FCC_A1#1,MO)
6:T-273.15,W(FCC_A1#1,SI)
7:T-273.15,W(FCC_A1#1,V)
8:T-273.15,W(FCC_A1#1,W)

THERMO-CALC (2009.04.15:02.59) :example 8d
DATABASE:TCFE6
W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2,
W(V)=2E-2, P=1E5, N=1.;



9

Calculation of Dew Point

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of dew point
SYS: @@
SYS:
SYS: go data
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw psub
 Current database: TCS Public Pure Substances TDB v1

 VA  DEFINED
TDB_PSUB: def-sp h2 h2o1
 H2                      H2O1  DEFINED
TDB_PSUB: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous species, stoichiometric solids and
      liquids in the Cu-Fe-H-N-O-S system.'
 -OK-
TDB_PSUB: go p-3
 POLY version  3.32,  Dec 2007
POLY_3: s-c n=1 p=1e5 t=233
POLY_3: ch-st ph h2o_l=f 0
POLY_3: c-e
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          138  grid points in            0  s
    22 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
 Output from POLY-3, equilibrium =     1, label A0  , database: PSUB

 Conditions:
 N=1, P=1E5, T=233
 FIXED PHASES
 H2O_L=0
 DEGREES OF FREEDOM 0

 Temperature    233.00 K (   -40.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00931E+00
 Total Gibbs energy -1.53589E+04,  Enthalpy -9.53654E+02,  Volume  9.68549E-03

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 H                       9.9991E-01  9.9851E-01 3.6499E-04 -1.5335E+04 SER
 O                       9.3928E-05  1.4889E-03 1.0377E-61 -2.7203E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0093E+00, Volume fraction 1.0000E+00  Mass fractions:
 H  9.98511E-01  O  1.48890E-03
 Constitution:
 H2    9.99812E-01  H2O1  1.87874E-04

 H2O_L                       Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O  8.88103E-01  H  1.11897E-01
```

```
POLY_3: ent fun ph2_h2o=acr(h2,gas)/acr(h2o,gas);
POLY_3: s-a-v 1 t 173.15 373.15 ,
POLY_3: save dew y
POLY_3: step,,
 No initial equilibrium, using default
 Step will start from axis value    233.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

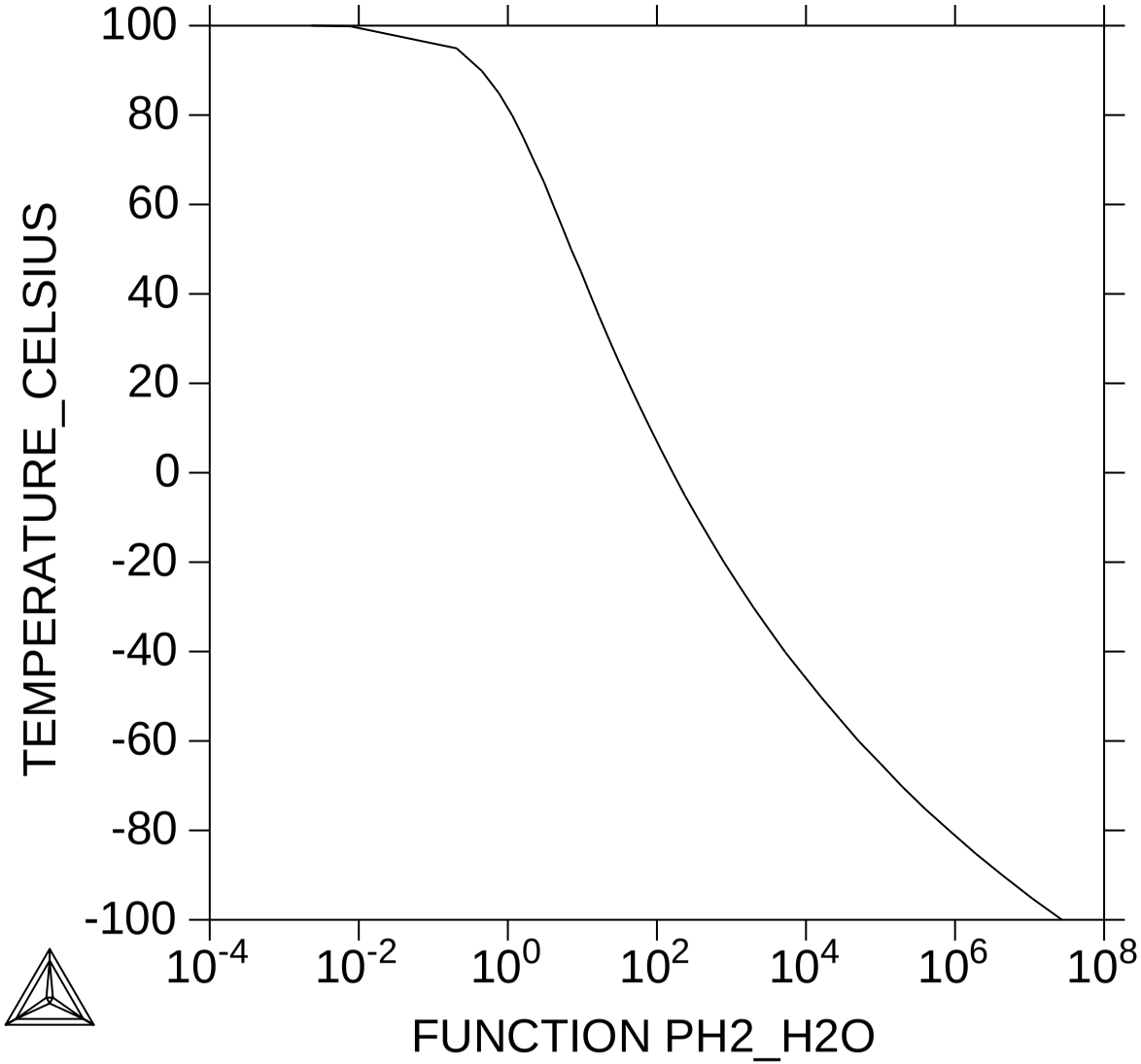
 Phase Region from    233.000     for:
     GAS
     H2O_L
 Global test at  2.73000E+02 .... OK
 Global test at  3.23000E+02 .... OK
 Global test at  3.73000E+02 .... OK
 Terminating at    373.150
 Calculated    32 equilibria

 Phase Region from    233.000     for:
     GAS
     H2O_L
 Global test at  1.93000E+02 .... OK
 Terminating at    173.150
 Calculated    15 equilibria
 *** Buffer saved on file: dew.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x ph2_h2o
POST: s-a-ty x log
POST: s-d-a y t-c
POST: pl
POST:
POST:
POST: set-inter
POST:POST: CPU time           0  seconds
```

THERMO-CALC (2009.04.15:02.59) :
DATABASE:PSUB
N=1., P=1E5, FIXED PHASES: H2O_L=0;



10

Preventing clogging of Cr_2O_3 in a continuous casting process

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example showing how to avoid clogging
SYS: @@ in a continuous casting process
SYS: @@
SYS: @@ The background to this example is that a manufacturer wanted
SYS: @@ to increase the Cr content of a material from 18 to 25 weight
SYS: @@ percent. He then had trouble in the continous casting of this
SYS: @@ material because solid Cr2O3 was formed. By calculating the
SYS: @@ equilibria in the steel/slag system a simple correction could
SYS: @@ be found: modify the Mn or Si content, thus decrease the oxygen
SYS: @@ potential.
SYS: @@ In Thermo-calc, one can FIX a phase with zero amount to simulate
SYS: @@ how to avoid forming this phase. One should then release one of the
SYS: @@ conditions, usually one of the compositions, and this composition
SYS: @@ is determined by the equilibrium calculation.
SYS: @@
SYS: set-log ex10,,,,
SYS: @@ The user goes to the database module to obtain data
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: @@ Switch to the database with slag data
TDB_TCFE6: sw slag2
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Fe-containing Slag Database v2

 FE                      O  DEFINED
TDB_SLAG2: @@ Some information about the database is given by this command
TDB_SLAG2: d-i
   ... the command in full is DATABASE_INFORMATION
 Current database: TCS Fe-containing Slag Database v2

                SLAG2 -- TC Fe-containing Slag Database
          ************************************************
                          (Version 2.2, June 2006)

      Copyright @ 1992-2006: Thermo-Calc Software, Stockholm, Sweden

   This updated SLAG2 Slag Database contains a liquid slag phase, as well
     as an Fe-rich liquid phase (dilute solution), a pure FeO liquid phase,
     a large gaseous mixture phase, and many stoichiometric solids and
     solid solution phases (e.g., oxides, silicates, sulfides, phosphates,
     halites, etc.), within a wide chemical framework of 30 elements:
         Ag    Al    Ar    B     C     Ca    Co    Cr    Cu    F
         Fe    H     Mg    Mn    Mo    N     Na    Nb    Ni    O
         P     Pb    S     Si    Sn    Ti    U     V     W     Zr
   Thermodynamic data for the liquid slag phase and oxide/silicate solid
     phases in the Al2O3-CaO-CrO-Cr2O3-FeO-Fe2O3-MgO-MnO-Na2O-SiO2 system
     were critically assessed by IRSID (1984), using the Kapoor-Frohberg-
     Gaye Quasichemical Cell Model, i.e., the Kapoor-Frohberg Slag Model
     with the extensions introduced by Gaye and Welfringer (1984) for
     complex multicomponent slag solution systems.
   Data for the additional components S, P and F (as sulfide, phosphate
     and fluoride species in the framework of [Al+3, Ca+2, Cr+2, Cr+3,
     Fe+2, Fe+3, Mg+2, Mn+2, Na+, Si+4, P+5, (PO)+3, O-2, S-2, and F-]
     in the slag phase and some S-/P-/F-bearing solid phases, which were
     critically assessed by IRSID (1997), have been added to the database,
     and it thus allows calculations of sulfide capacities of liquid slag.
   Note that composition-dependent parameters in solid solution phases have
     not been considered in this particular database.
```

Data for a dilute solution of many elements in the Fe-rich liquid phase are critically assessed and converted to regular solution parameters according to Hillert (1986), with modified dilute solution parameters (plus a quadratic term) in Fe-rich liquid from Sigworth and Elliot (1974), so that it becomes a consistent thermodynamic model and also generally improves the agreements of calculated results with available experimental data. The following 26 dilute components are included in the FE-Liquid solution phase:
Ag Al B C Ca Co Cr Cu H Mg Mn Mo N Nb Ni O P Pb S Si Sn Ti U V W Zr
Data are evaluated at infinite dilution and the recommended composition limit of any minority component, in the 27-component diluted Fe-rich liquid, is only 0.1wt%. In some cases, data could be used at much higher concentrations in the Fe-rich liquid phase, but the user must carefully check each of such cases.

The database is suitable for activity and phase equilibrium calculations in metallurgical slag systems containing iron.

The first release (SLAG) was in 1992, and the last modification was made in 1998. In this updated version (SLAG2 of 2002), many thermodynamic parameters for the slag phase, Fe-rich liquid phase, and various solid phases have been improved and implemented, and a greatly enlarged phase description and thermodynamic properties for the gaseous mixture phase (within the framework of all the covered 30 elements) has been included.

For steels and various alloys, as well as other substance or solution phases, which are in interactions with the Fe-rich liquid phase or the liquid slag phase, thermodynamic data can be appended from other available databases, such as TCFE, TCNI, SSUB, SSOL, SALT, TCMP, TCES, TTAL/MG/NI/TI, TCAQ, AQS, GCE, NUMT, NUOX, etc. For more information on such databases, please consult Thermo-Calc Software.

Release History: Version 1.0 initial release, 1992
Version 1.1 with minor improvements, 1998
Version 2.0 with major improvements, 2002
Version 2.1 with major improvements, 2003
Version 2.2 with minor improvements, 2006

Edited by: Bo Sundman & Pingfang Shi (Thermo-Calc Software, Sept 2006).

TDB_SLAG2: **@?<Hit_return_to_continue>**
TDB_SLAG2: ***@@ The user defines his system by giving the elements. Note that Fe***
TDB_SLAG2: ***@@ and O are included by default.***
TDB_SLAG2: **d-sys mn si cr al**
... the command in full is DEFINE_SYSTEM
MN SI CR
AL DEFINED
TDB_SLAG2: ***@@ 'GET' reads thermodynamic data from the database files to the***
TDB_SLAG2: ***@@ program***
TDB_SLAG2: **get**
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES ......
PHASES ....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'SLAG2 (2006): TCS Fe-Containing Slag Database, V2.2, owned and provided by Thermo-Calc Software.'
'TCMP2 (2004): TCS Materials Processing Database, V2.3, owned and provided by Thermo-Calc Software.'
-OK-
TDB_SLAG2:
TDB_SLAG2: **go p-3**
... the command in full is GOTO_MODULE

POLY version 3.32, Dec 2007
POLY_3:
POLY_3: ***@@ There are many commands in the POLY-3 module***
POLY_3: **?**
... the command in full is HELP

ADD_INITIAL_EQUILIBRIUM	EXIT	REINITIATE_MODULE
ADVANCED_OPTIONS	GOTO_MODULE	SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA	HELP	SELECT_EQUILIBRIUM
BACK	INFORMATION	SET_ALL_START_VALUES
CHANGE_STATUS	LIST_AXIS_VARIABLE	SET_AXIS_VARIABLE

```
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS          SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM         SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA  SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS              SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS             SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN          SET_START_VALUE
 DELETE_SYMBOL            MAP                      SHOW_VALUE
 ENTER_SYMBOL             POST                     STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES          TABULATE
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Some basic information is given by the INFORMATION command
POLY_3: @@ Look at example 1 for more details.
POLY_3: info
   ... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/:  ?
 WHICH SUBJECT

 Specify a subject (or its abbreviation as long as it is unique, e.g.,
 SIN, SIT, SOL, SPE, STATE, STEP, SYM, SYS, SUB, etc.) on which information
 should be given, from the following subjects that are important to the use
 of the POLY module:

  PURPOSE                 GETTING STARTED          USER INTERFACE
  HELP                    MACRO FACILITY           PRIVATE FILES
  BASIC THERMODYNAMICS    SYSTEM AND PHASES        CONSTITUENTS AND SPECIES
  SUBLATTICES             COMPONENTS               SITE AND MOLE FRACTIONS
  COMPOSITION AND CONSTITUTION                     CONCENTRATION
  STATE VARIABLES         INTENSIVE VARIABLES      EXTENSIVE VARIABLES
  DERIVED VARIABLES       UNITS                    BASIC UNITS
  SYSTEM UNITS            COMPONENT UNITS          PHASE UNITS
  PHASE-COMPONENT UNITS   PHASE-SPECIES UNITS      USER-SPECIFIED UNITS
  SYMBOLS                 REFERENCE STATES         METASTABLE EQUILIBRIUM
  CONDITIONS              AXIS-VARIABLES           SPECIAL OPTIONS
  CALCULATIONS TYPES      SINGLE EQUILIBRIUM       INITIAL EQUILIBRIUM
  STEPPING                SOLIDIFICATION PATH      PARAEQUILIBRIUM AND T0
  MAPPING                 PLOTTING OF DIAGRAMS     GLOBAL MINIMIZATION
  DIAGRAM TYPES           BINARY DIAGRAMS          TERNARY DIAGRAMS
  QUASI-BINARY DIAGRAMS   HIGHER ORDER DIAGRAMS    PROPERTY DIAGRAMS
  POTENTIAL DIAGRAMS      POURBAIX DIAGRAMS        AQUEOUS SOLUTIONS
  ORDER-DISORDER          TROUBLE SHOOTING         FAQ

 If you are using the ED_EXP module (the sub-module of the PARROT module),
 you can also get detailed information of the following subject keywords
 which are relevant to the EX_EXP module:

  EDEXP     for Edit-Experiment Module (ED-EXP)
  EDPOLY    for Performance of POLY Commands in the ED_EXP Module
  EDSPECIAL for Special Commands only available in the ED_EXP Module
  EDPOP     for Other Commands in the Experimental Data (POP or DOP) Files

WHICH SUBJECT /PURPOSE/:
 PURPOSE

          INTRODUCTION to the Equilibrium Calculation Module (POLY)
         ***********************************************************

 Knowledge of the thermodynamic equilibrium is an important factor for
 understanding properties of materials and processes. With a database of
 thermodynamic model parameters, it is possible to predict such properties
 and also to obtain driving forces for diffusion-controlled phase
 transformations and other dynamic processes.

 With the comprehensive Equilibrium Calculation module, POLY ? it is possible
 to calculate many different kinds of equilibria and diagrams, in particular
 multicomponent phase diagrams. This is thus an important tool in developing
 new materials and processes. The current POLY module is its third version;
 this is why is often referred as POLY_3 in the Thermo-Calc software.

 Different kind of databases can be used with the POLY module, and thus it
 can be used for alloys or ceramic system, as well as gaseous equilibria,
 aqueous solution involved heterogeneous interaction systems. Since TCCN,
 up to 40 elements and 1000 species can be defined into a single system
 (previously 20 elements and 400 species) for equilibrium calculations.
```

Great care has been taken to provide the users with the most flexible tool. All normal thermodynamic state variables can be used to set as conditions in calculating equilibria, and as axes in plotting diagrams. A unique facility is to set the composition or any property of an individual phase as a condition. Any state variable can be varied along an axis in order to generate a diagram. During calculations of a diagram, complete descriptions of all calculated equilibria are stored, and in the diagram any state variable can be used as axis.

One of the major improvements since the TCCR/TCW4 software version is that the recently-implemented Global Minimization Technique is used to assure that the present minimum in an equilibrium calculation is the most stable minima for the specified conditions. This new technique, which is based on the traditional GEM (Gibbs Energy Minimization) Technique (i.e., the ordinary POLY Minimization routines used in previous versions, where pre-knowledge of miscibility gaps in involved phases are necessary, otherwise, metastable equilibria instead of the stable equilibria may be obtained), will ultimately prevent a calculation from reaching an undesired metastable or unstable (local) equilibrium in a defined system, and automatically detect possible miscibility gap(s) and automatically create additional composition sets in a solution phase if needed for handling single or multiple miscibility gaps. Therefore it is no longer necessary for the user to specify additional composition sets in advance.

A Direct Global Minimization can be performed on conditions: N, n(comp), B, b(comp), w(comp), x(comp), T, and P, but not when combined conditions as e.g. w(a)-3*w(b)=1 are used or when an activity or potential condition is used. For all other types of conditions where regular minimization converges, Indirect Global Minimization, i.e. global test and corrections, if necessary, are performed until the lowest minimum is found.

 * Direct Global Minimization: From the mesh of Gibbs energy, find the set of grid points that gives the lowest energy solution under the specified conditions. This set of grid points provides starting combination of phases and their constitutions for regular minimization to find the exact equilibrium solution. This solution will be then subject to a global test as described below.

 * Indirect Global Minimization: Under certain conditions, direct approach is impossible. In this case, regular minimization is performed first and then a check is performed in order to see if the found local minimum is a global one by checking if all grid points are above the equilibrium Gibbs energy plane. If not, then recalculate by including these grid points until no grid point is above the equilibrium Gibbs energy plane from the previous step.

The full-scale and full-scope usage of the Global Minimization Technique has been extended from for only single-point calculations within TCCR/TCW4 to for all types of calculations (of single-points, property diagram stepping and phase diagram mapping) within TCCS/TCW5.

The use of Global Minimization Technique may increase the computation time, while it is not an issue at all, thanks for the rapid developments of computer hardware nowadays.

 * The main cost in time comes from the calculation of Gibbs energy at each grid point generated by properly meshing the composition space for each entered phase. In a typical multicomponent system calculation, about 100MB of RAM memory is needed in storing the mesh of Gibbs energies.

 * An additional (but much smaller) cost in time comes from finding the set of grid points in the above mesh that give the lowest energy solution. This solution is where POLY starts its ordinary minimization. When POLY has found an equilibrium, the equilibrium Gibbs energy surface is compared to the mesh to assure that no grid point is below the surface, i.e. a global minimization has been reached.

Global Minimization is now performed by default in single-point or stepping or mapping equilibrium calculations, but can of course be turned off (and on again by repeating the command-sequence of ADVANCED_OPTIONS GLOBAL_MINIMIZATION) by the user for specific purposes. This means that truly stable equilibrium should be guaranteed for single-points, stepping and mapping calculations.

* A completely new stepping and mapping procedure that ensures Global Minimization everywhere it is critical has been developed and been made available in TCCS/TCW5. These newly re-written STEP/MAP routines are very important for stepping/mapping calculations in multicomponent systems where there are complex miscibility gaps in some phases, and it does not require having any ¡°good¡± guess of starting points. Therefore, TCCS/TCW5 can automatically handle complex solution phases with single or multiple miscibility gaps [for instance, a solution phase that is thermodynamically described as a single phase in a Thermo-Calc database, such as FCC, BCC or HCP phases, may be split into two or several composition-sets/phases that are presented in an equilibrium state as metallic phase(s), carbide(s), nitride(s), carbonitride(s), nitrocarbide(s), and so on], and can thus ensure the correct and complete phase diagrams and property diagrams in multicomponent systems, without bothering staring points.

Together with the PARROT module, the POLY module is also used for critical assessment of experimental data in order to develop thermodynamic databases. The POLY module uses the Gibbs Energy System (GES) for modeling and data manipulations of the thermodynamic properties of each phase.

The following commands are available in the POLY module:

```
POLY_3:?
 ADD_INITIAL_EQUILIBRIUM  EXIT                      REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE               SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                      SELECT_EQUILIBRIUM
 BACK                     INFORMATION               SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE        SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS           SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM          SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA   SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS               SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS              SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM  SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN           SET_START_VALUE
 DELETE_SYMBOL            MAP                       SHOW_VALUE
 ENTER_SYMBOL             POST                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES           TABULATE
POLY_3:
```

Note that, since TCCS, the SPECIAL_OPTIONS and SET_MINIMIZAION_OPTIONS commands (the later one was introduced in the TCCR version) has been merged into the new ADVANCED_OPTIONS command; and the RECOVER_START_VALUES command has been removed, due to that is not relevant to the POLY module anymore.

Revision History of the POLY-Module User’s Guide:

```
================================================
 Mar 1991  First release
                   (Edited by Bo Jansson and Bo Sundman)
 Oct 1993  Second revised release (with version J)
                   (Edited by Bo Jansson and Bo Sundman)
 Oct 1996  Third revised release (with version L)
                   (Edited by Bo Sundman)
 Nov 1998  Fourth revised release (with version M)
                   (Edited by Bo Sundman)
 Jun 2000  Fifth revised and extended release
                   (Edited by Pingfang Shi)
 Nov 2002  Sixth revised and extended release
                   (Edited by Pingfang Shi)
 May 2006  Eighth revised and extended release
                   (Edited by Pingfang Shi)
 Apr 2008  Ninth revised and extended release
                   (Edited by Pingfang Shi)
```

```
WHICH SUBJECT:
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Now set the conditions i.e. the temperature, pressure and
POLY_3: @@ composition. We are interested in the situation at the
POLY_3: @@ outflow of steel
POLY_3: s-c t=1800,p=101325,n=1
   ... the command in full is SET_CONDITION
POLY_3: @@ As conditions one can specify that the steel should have
POLY_3: @@ 18 weight percent of Cr, 0.4 w/o Mn and 0.4 w/o Si
POLY_3: @@ (Note that the overall amount of Cr and Mn is not specified).
```

```
POLY_3: s-c w(mn)=.004,w(cr)=.18,w(si)=.004
   ... the command in full is SET_CONDITION
POLY_3: @@ The amount of Al is very small, assume 5 ppm
POLY_3: s-c w(al)=5e-6
   ... the command in full is SET_CONDITION
POLY_3: @@ We will later assume that the oxygen potential is determined
POLY_3: @@ by the equilibrium with liquid slag but initially we assume
POLY_3: @@ there is 100 ppm O
POLY_3: s-c w(o)=1e-4
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=5E-6,
    W(O)=1E-4
 DEGREES OF FREEDOM 0
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Let us check what phases we have
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 WUSTITE                ENTERED    0.00000000E+00  0.00000000E+00
 SIO2                   ENTERED    0.00000000E+00  0.00000000E+00
 SI2O4_AL6O9            ENTERED    0.00000000E+00  0.00000000E+00
 MNO_SIO2               ENTERED    0.00000000E+00  0.00000000E+00
 MNO_AL2O3              ENTERED    0.00000000E+00  0.00000000E+00
 MNO                    ENTERED    0.00000000E+00  0.00000000E+00
 MN2O2_SIO2             ENTERED    0.00000000E+00  0.00000000E+00
 FEO_AL2O3              ENTERED    0.00000000E+00  0.00000000E+00
 FEOLIQ                 ENTERED    0.00000000E+00  0.00000000E+00
 FE2O3                  ENTERED    0.00000000E+00  0.00000000E+00
 FE2O2_SIO2             ENTERED    0.00000000E+00  0.00000000E+00
 CR2O3                  ENTERED    0.00000000E+00  0.00000000E+00
 AL2O3                  ENTERED    0.00000000E+00  0.00000000E+00
 SLAG                   ENTERED    0.00000000E+00  0.00000000E+00
 FE_LIQUID              ENTERED    0.00000000E+00  0.00000000E+00
 GAS                    ENTERED    0.00000000E+00  0.00000000E+00
POLY_3: @@ We start by assuming all other phases except FE_LIQUID are suspended
POLY_3: ch-st p *
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:  sus
POLY_3: ch-st p fe-l=ent
   ... the command in full is CHANGE_STATUS
Start value, number of moles /0/:  0
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=5E-6,
    W(O)=1E-4
 DEGREES OF FREEDOM 0
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The degree of freedoms is zero and we can make a calculation.
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated           20  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ Now set the suspended phases as dormant
POLY_3: c-st p *s=d
   ... the command in full is CHANGE_STATUS
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated           20  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 FE_LIQUID              ENTERED    0.00000000E+00  1.00000000E+00
 AL2O3                  DORMANT   -1.37900950E-01
 SI2O4_AL6O9            DORMANT   -1.39085603E-01
 SLAG                   DORMANT   -1.41634170E-01
```

```
 MNO_AL2O3               DORMANT   -2.58619718E-01
 CR2O3                   DORMANT   -3.21091035E-01
 FEO_AL2O3               DORMANT   -4.73834466E-01
 SIO2                    DORMANT   -4.97094549E-01
 MNO_SIO2                DORMANT   -5.72185921E-01
 MN2O2_SIO2              DORMANT   -6.74259142E-01
 FE2O2_SIO2              DORMANT   -1.35589759E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN -1.45362622E+00
 MNO FEOLIQ WUSTITE FE2O3 GAS
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ If the stable phases do not change in 12 iterations the program
POLY_3: @@ terminates even if the program has not calculated the correct
POLY_3: @@ driving forces for the metastable phases.
POLY_3: @@ You can change that and other things by the command SET-NUMERICAL-LIMITS
POLY_3: @@ We now use that to change the lowest value of a fraction variable.
POLY_3: s-n-l
   ... the command in full is SET_NUMERICAL_LIMITS
 LIMITATIONS of the present version of Thermo-Calc
 Max number of elements                      :  40
 Max number of species                       :1000
 Max number of sublattices in a phase        :  10
 Max number of constituents in a phase:      : 200
 Max number of constituents in an ideal phase :1000

Maximum number of iterations /500/:  500
Required accuracy /1E-06/:  1E-6
Smallest fraction /1E-12/:  1E-12
Approximate driving force for metastable phases /Y/:  n
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Calculate once more
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FE_LIQUID               ENTERED    0.00000000E+00  1.00000000E+00
 AL2O3                   DORMANT   -1.37900950E-01
 SI2O4_AL6O9             DORMANT   -1.39085603E-01
 SLAG                    DORMANT   -1.41634242E-01
 MNO_AL2O3               DORMANT   -2.58619718E-01
 CR2O3                   DORMANT   -3.21091035E-01
 FEO_AL2O3               DORMANT   -4.73834466E-01
 SIO2                    DORMANT   -4.97094549E-01
 MNO_SIO2                DORMANT   -5.72185921E-01
 MN2O2_SIO2              DORMANT   -6.74259142E-01
 FE2O2_SIO2              DORMANT   -1.35589759E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN -1.45362622E+00
 MNO FEOLIQ WUSTITE FE2O3 GAS
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The driving forces are quite stable.
POLY_3: @@ Now set the slag phase stable and let the program
POLY_3: @@ adjust the amount of oxygen to make it stable
POLY_3: c-st p slag=fix 0
   ... the command in full is CHANGE_STATUS
POLY_3: s-c w(o)
   ... the command in full is SET_CONDITION
Value /1E-04/:  none
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=5E-6
 FIXED PHASES
 SLAG=0
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          426  grid points in           0  s
    91 ITS,  CPU TIME USED  18 SECONDS
```

```
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG2

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=5E-6
 FIXED PHASES
 SLAG=0
 DEGREES OF FREEDOM 0

 Temperature   1800.00 K (  1526.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.48772E+01
 Total Gibbs energy -1.12619E+05,  Enthalpy  7.09970E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      1.0169E-05  5.0000E-06 1.4560E-10 -3.3899E+05 SER
 CR                      1.8997E-01  1.8000E-01 5.0814E-04 -1.1351E+05 SER
 FE                      7.9777E-01  8.1187E-01 6.2367E-04 -1.1045E+05 SER
 MN                      3.9956E-03  4.0000E-03 2.3982E-06 -1.9367E+05 SER
 O                       4.3479E-04  1.2676E-04 4.3110E-13 -4.2612E+05 SER
 SI                      7.8159E-03  4.0000E-03 4.4707E-08 -2.5327E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4877E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.11868E-01  SI  4.00000E-03  O   1.26759E-04
 CR  1.80000E-01  MN  4.00000E-03  AL  5.00000E-06

 SLAG                        Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   4.05346E-01  MN  1.66460E-01  CR  9.18504E-02
 AL  2.10106E-01  SI  1.06467E-01  FE  1.97705E-02
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ List also the status of the phases.
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 SLAG                    FIXED      0.00000000E+00  0.00000000E+00
 FE_LIQUID               ENTERED    0.00000000E+00  1.00000000E+00
 SI2O4_AL6O9             DORMANT   -5.64799855E-03
 AL2O3                   DORMANT   -1.38163583E-02
 MNO_AL2O3               DORMANT   -1.36363415E-01
 CR2O3                   DORMANT   -1.79788767E-01
 SIO2                    DORMANT   -3.40274413E-01
 FEO_AL2O3               DORMANT   -3.51488184E-01
 MNO_SIO2                DORMANT   -4.31019607E-01
 MN2O2_SIO2              DORMANT   -5.39801608E-01
 FE2O2_SIO2              DORMANT   -1.22126010E+00
 MNO                     DORMANT   -1.33594064E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN -1.92533191E+00
 FEOLIQ WUSTITE FE2O3 GAS
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Note that mullite and corundum are almost stable!
POLY_3: @@ The amount of Al is probably too high, set it
POLY_3: @@ to half of the initial value
POLY_3: s-c w(al)
   ... the command in full is SET_CONDITION
Value /5E-06/:  2.5e-6
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    84 ITS,  CPU TIME USED  16 SECONDS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 SLAG                    FIXED      0.00000000E+00  0.00000000E+00
 FE_LIQUID               ENTERED    0.00000000E+00  1.00000000E+00
 CR2O3                   DORMANT   -6.84853495E-02
 SI2O4_AL6O9             DORMANT   -1.00726657E-01
```

```
 AL2O3                     DORMANT   -1.96319655E-01
 SIO2                      DORMANT   -2.16791477E-01
 MNO_AL2O3                 DORMANT   -2.40246383E-01
 MNO_SIO2                  DORMANT   -3.19862705E-01
 MN2O2_SIO2                DORMANT   -4.33927292E-01
 FEO_AL2O3                 DORMANT   -4.55278108E-01
 FE2O2_SIO2                DORMANT   -1.11519970E+00
 MNO                       DORMANT   -1.24327279E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN -1.83233841E+00
 FEOLIQ WUSTITE FE2O3 GAS
POLY_3: @@ The Al2O3 phases are now less close to be stable.
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG2

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=2.5E-6
 FIXED PHASES
 SLAG=0
 DEGREES OF FREEDOM 0

 Temperature   1800.00 K (  1526.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.48739E+01
 Total Gibbs energy -1.12645E+05,  Enthalpy  7.09808E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      5.0843E-06  2.5000E-06 6.9805E-11 -3.4999E+05 SER
 CR                      1.8996E-01  1.8000E-01 5.0782E-04 -1.1352E+05 SER
 FE                      7.9770E-01  8.1185E-01 6.2371E-04 -1.1045E+05 SER
 MN                      3.9953E-03  4.0000E-03 2.3968E-06 -1.9368E+05 SER
 O                       5.2292E-04  1.5246E-04 5.1918E-13 -4.2334E+05 SER
 SI                      7.8154E-03  4.0000E-03 4.4645E-08 -2.5329E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4874E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.11845E-01  SI  4.00000E-03  O   1.52461E-04
 CR  1.80000E-01  MN  4.00000E-03  AL  2.50000E-06

 SLAG                        Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   3.98382E-01  SI  1.47882E-01  CR  9.38151E-02
 MN  2.04453E-01  AL  1.36163E-01  FE  1.93041E-02
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ We assume that this describes the situation at 18 w/o Cr. Some
POLY_3: @@ liquid slag that later will form mainly SiO2-Al2O3-MnO is present.
POLY_3: @@ Now increase the Cr-content to 25 w/o
POLY_3: s-c w(cr)
   ... the command in full is SET_CONDITION
Value /.18/:  .25
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    92 ITS,  CPU TIME USED  18 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG2

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=2.5E-6
 FIXED PHASES
 SLAG=0
 DEGREES OF FREEDOM 0

 Temperature   1800.00 K (  1526.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45790E+01
 Total Gibbs energy -1.12766E+05,  Enthalpy  7.08286E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      5.0570E-06  2.5000E-06 5.6802E-11 -3.5307E+05 SER
 CR                      2.6242E-01  2.5000E-01 6.9387E-04 -1.0885E+05 SER
 FE                      7.2488E-01  7.4172E-01 5.6877E-04 -1.1183E+05 SER
 MN                      3.9739E-03  4.0000E-03 2.5527E-06 -1.9274E+05 SER
```

```
 O                      9.4994E-04  2.7846E-04 5.2027E-13 -4.2331E+05 SER
 SI                     7.7734E-03  4.0000E-03 4.4234E-08 -2.5343E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4579E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  7.41719E-01  SI  4.00000E-03  O   2.78462E-04
 CR  2.50000E-01  MN  4.00000E-03  AL  2.50000E-06

 SLAG                        Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   3.75965E-01  CR  1.46858E-01  AL  1.08555E-01
 MN  2.29782E-01  SI  1.22510E-01  FE  1.63299E-02

 CR2O3                       Status DORMANT     Driving force  5.7637E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CR  6.84207E-01  AL  0.00000E+00  FE  0.00000E+00
 O   3.15793E-01  MN  0.00000E+00  SI  0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Now Cr2O3 would like to be stable. The simplest correction is to modify
POLY_3: @@ the composition of the steel in order to decrease the oxygen potential.
POLY_3: @@ For example the Mn or Si content could be changed.
POLY_3: @@ In order to determine which of these has the largest influence
POLY_3: @@ on the oxygen potential, calculate this by the partial derivative
POLY_3: @@ of the oxygen activity w.r.t. the Mn and Si content.
POLY_3: s-ref-s o gas
   ... the command in full is SET_REFERENCE_STATE
Temperature /*/:
Pressure /1E5/:
POLY_3: show acr(o)
   ... the command in full is SHOW_VALUE
 ACR(O)=7.6211754E-7
POLY_3: show acr(o).w(mn)
   ... the command in full is SHOW_VALUE
 ACR(O).W(MN)=-3.8683235E-5
POLY_3: show acr(o).w(si)
   ... the command in full is SHOW_VALUE
 ACR(O).W(SI)=-4.3891272E-5
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The value is largest for Si and thus the smallest change is necessary
POLY_3: @@ for that. Instead of modifying this content in steps one may
POLY_3: @@ specify that the Cr2O3 phase should be on its limit of stability, i.e.
POLY_3: @@ set it FIX with zero amount and calculate the change in composition.
POLY_3: c-s p cr2o3
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:  fix
Number of moles /0/:  0
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=2.5E-6
 FIXED PHASES
 SLAG=0      CR2O3=0
 DEGREES OF FREEDOM -1
POLY_3: s-c w(si)
   ... the command in full is SET_CONDITION
Value /.004/:  none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          427  grid points in            0  s
    88 ITS,  CPU TIME USED  17 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG2

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(AL)=2.5E-6
 FIXED PHASES
 SLAG=0      CR2O3=0
 DEGREES OF FREEDOM 0

 Temperature   1800.00 K (  1526.85 C),  Pressure  1.013250E+05
```

```
 Number of moles of components  1.00000E+00,  Mass in grams  5.44917E+01
 Total Gibbs energy -1.13206E+05,  Enthalpy  7.04662E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      5.0489E-06  2.5000E-06 5.9198E-11 -3.5245E+05 SER
 CR                      2.6200E-01  2.5000E-01 6.9265E-04 -1.0888E+05 SER
 FE                      7.2208E-01  7.4004E-01 5.6625E-04 -1.1189E+05 SER
 MN                      3.9675E-03  4.0000E-03 2.6126E-06 -1.9239E+05 SER
 O                       9.0829E-04  2.6668E-04 6.9312E-07 -2.1225E+05 GAS
 SI                      1.1038E-02  5.6888E-03 6.5541E-08 -2.4755E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4492E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  7.40042E-01  SI  5.68880E-03  O   2.66678E-04
 CR  2.50000E-01  MN  4.00000E-03  AL  2.50000E-06

 SLAG                        Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   3.99712E-01  SI  1.70607E-01  CR  9.75921E-02
 MN  2.11039E-01  AL  1.05909E-01  FE  1.51403E-02

 CR2O3                       Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CR  6.84207E-01  AL  0.00000E+00  FE  0.00000E+00
 O   3.15793E-01  MN  0.00000E+00  SI  0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ We can read the new Si content from this list but also
POLY_3: @@ show the value of a variable directly
POLY_3: SH W(SI)
   ... the command in full is SHOW_VALUE
 W(SI)=5.6888046E-3
POLY_3: @@ We have to increase the Si content to almost 0.6 w/o to avoid
POLY_3: @@ forming Cr2O3. Calculate also how much the Mn content must be changed
POLY_3: s-c w(si)
   ... the command in full is SET_CONDITION
Value /.005688804632/:  .004
POLY_3: s-c w(mn)
   ... the command in full is SET_CONDITION
Value /.004/:  none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    87 ITS,  CPU TIME USED  16 SECONDS
POLY_3: sh w(mn)
   ... the command in full is SHOW_VALUE
 W(MN)=6.0678237E-3
POLY_3: @@ Check with Si content equal to 0.5. It should be consistent with
POLY_3: @@ the plot below, i.e. Mn content decreases with increasing Si content.
POLY_3: s-c w(si)=.005
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    81 ITS,  CPU TIME USED  16 SECONDS
POLY_3: sh w(mn)
   ... the command in full is SHOW_VALUE
 W(MN)=4.8422333E-3
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Plot how the Mn content varies when the Si content
POLY_3: @@ varies between 0.2 and 0.8 w/o.
POLY_3: s-a-v 1 w(si)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0.002
Max value /1/:  0.008
Increment /1.5E-04/:  0.0004
POLY_3: save tcex10 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
```

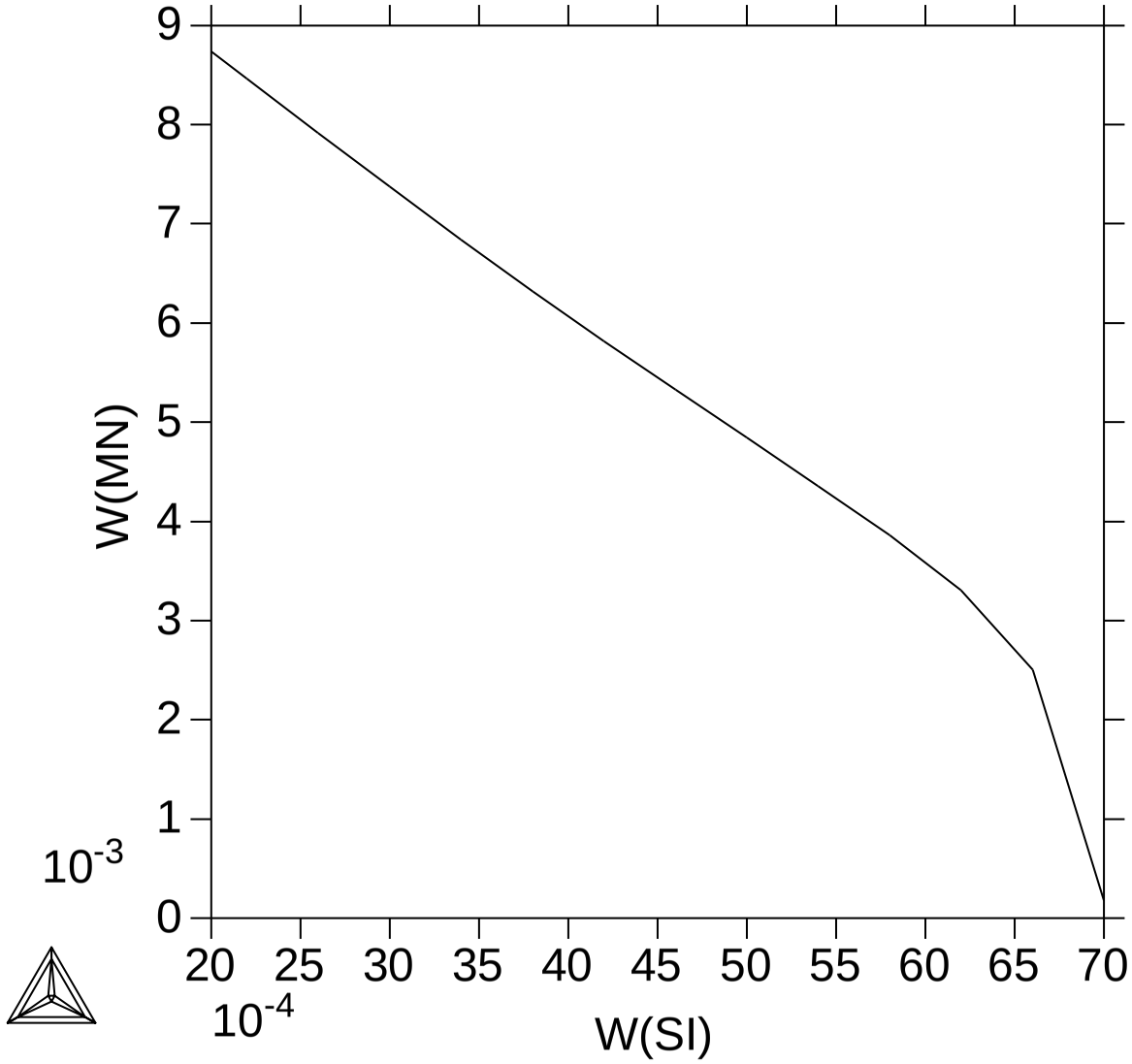
```
 No initial equilibrium, using default
 Step will start from axis value   0.500000E-02
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from   0.500000E-02 for:
     FE_LIQUID
     SLAG
     CR2O3
 QBSMER trying to find equilibrium at   7.0800000E-03
 QBSMER: Second global calculation
 Calculated     8 equilibria
 Sorry cannot continue  1717  55 1    7.0000000E-03

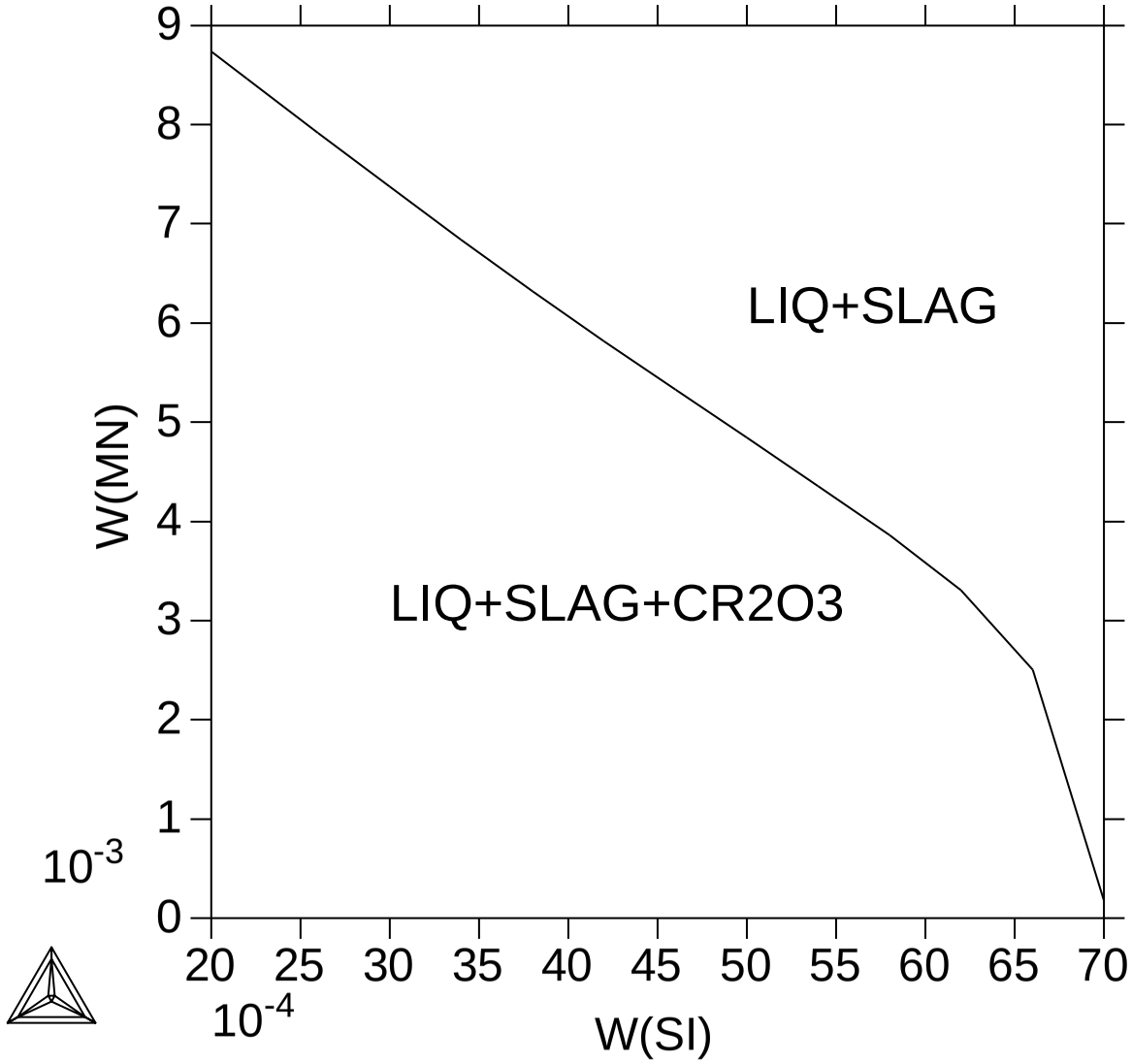
 Phase Region from   0.500000E-02 for:
     FE_LIQUID
     SLAG
     CR2O3
 Global test at  2.00000E-03 .... OK
 Terminating at   0.200000E-02
 Calculated    11 equilibria
 *** Buffer saved on file: tcex10.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-d-a x w(si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(mn)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: set-title example 10a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: add .005 .006 n
   ... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG
Text size: /.3999999762/:
POST: add .003 .003 n
   ... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG+CR2O3
Text size: /.3999999762/:
POST: set-title example 10b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time         144  seconds
```

THERMO-CALC (2009.04.15:03.02) :example 10a
DATABASE:SLAG2
T=1800, P=1.01325E5, N=1., W(CR)=0.25, W(AL)=2.5E-6 FIXED PHASES: SLAG=0CR2O3=



THERMO-CALC (2009.04.15:03.02) :example 10b
DATABASE:SLAG2
T=1800, P=1.01325E5, N=1., W(CR)=0.25, W(AL)=2.5E-6 FIXED PHASES: SLAG=0CR2O3=



11

Oxidation of Cu_2S with H_2O/O_2 gas

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Oxidation of Cu2S with H2O and O2 gas mixture
SYS: @@   Different O/H ratio represents different oxygen potential. Certain
SYS: @@   oxygen potential can desulphurize Cu2S without forming copper oxides.
SYS: @@   This example demonstrates how to find the optimum O/H ratio (i.e. oxygen
SYS: @@   potential).
SYS: @@   In Thermo-calc, the problem reduces to perform equilibria calculations in
SYS: @@   Cu-S-H-O system. The amounts of the components should be kept to correct
SYS: @@   ratio corresponding to Cu2S and H2O, by using a command SET_INPUT_
SYS: @@   AMOUNTS in POLY_3. Initially, O/H = 0.5 is given. Optimum O/H ratio
SYS: @@   is calculated by giving desired calculation conditions. For example,
SYS: @@   to simulate one phase disappearing, one can FIX the phase with zero amount
SYS: @@   in Thermo-calc.
SYS: @@
SYS: set-log ex11,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw
   ... the command in full is SWITCH_DATABASE
 Use one of these databases

 TCFE6   =  TCS Steels/Fe-Alloys Database v6
 TCFE5   =  TCS Steels/Fe-Alloys Database v5
 TCFE4   =  TCS Steels/Fe-Alloys Database v4
 TCFE3   =  TCS Steels/Fe-Alloys Database v3
 TCFE2   =  TCS Steels/Fe-Alloys Database v2
 TCFE1   =  TCS Steels/Fe-Alloys Database v1
 FEDAT   =  TCS/TT Steels Database v1
 TCNI1   =  TCS Ni-Alloys Database v1
 SSOL4   =  SGTE Alloy Solutions Database v4
 SSOL2   =  SGTE Alloy Solutions Database v2
 SBIN2   =  SGTE Binary Alloys Database v2
 SSUB4   =  SGTE Substances Database v4
 SPOT4   =  SGTE Potential Database v4
 SSUB3   =  SGTE Substances Database v3
 SPOT3   =  SGTE Potential Database v3
 SSUB2   =  SGTE Substances Database v2
 SPOT2   =  SGTE Potential Database v2
 SNOB1   =  SGTE Nobel Metal Alloys Database v2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1
 SALT1   =  SGTE Molten Salt Database v1
 SNUX6   =  SGTE In-Vessel Nuclear Oxide TDB v6.2
 SEMC2   =  TC Semi-Conductors Database v2
 SLAG2   =  TCS Fe-containing Slag Database v2
 SLAG1   =  TCS Fe-containing Slag Database v1
 ION2    =  TCS Ionic Solutions Database v2
 ION1    =  TCS Ionic Solutions Database v1
 NOX2    =  NPL Oxide Solutions Database, v2
 NSLD2   =  NPL Solder Alloys Database v2
 TCMP2   =  TCS Materials Processing Database v2
 TCES1   =  TCS Combustion/Sintering Database v1
 NUMT2   =  TCS Nuclear Materials Database v2
 NUOX4   =  TCS Nuclear Oxides Database v4
 NUTO1   =  TCS U-Zr-Si Ternary Oxides TDB v1
 NUTA1   =  TCS Ag-Cd-In Ternary Alloys TDB v1
 TCNF2   =  TCS Nuclear Fuels Database v2
 TTNI7   =  TT Ni-Alloys Database v7
 TTNI6   =  TT Ni-Alloys Database v6
 TTNI5   =  TT Ni-Alloys Database v5
```

```
 TTNF5   =  TT NiFe-Alloys Database v5
 TTTI3   =  TT Ti-Alloys Database v3
 TTTI2   =  TT Ti-Alloys Database v2
 TTTIAL  =  TT TiAl-Alloys Database v1
 TTAL6   =  TT Al-Alloys Database v6
 TTAL5   =  TT Al-Alloys Database v5
 TTAL4   =  TT Al-Alloys Database v4
 TTAL3   =  TTAL3setup.TDC TT Al-Alloys Database v3
 TTMG4   =  TT Mg-Alloys Database v4
 TTMG3   =  TT Mg-Alloys Database v3
 TTMG2   =  TT Mg-Alloys Database v2
 TTZR1   =  TT Zr-Alloys Database v1
 TCAQ2   =  TCS Aqueous Solution Database v2
 AQS2    =  TGG Aqueous Solution Database v2
 GCE2    =  TGG Geochemical/Environmental TDB v2
 CCC1    =  CCT Cemented Carbides Database v1
 PURE4   =  SGTE Unary (Pure Elements) TDB v4
 PSUB    =  TCS Public Pure Substances TDB v1
 PBIN    =  TCS Public Binary Alloys TDB v1
 PTERN   =  TCS Public Ternary Alloys TDB v1
 PKP     =  Kaufman Binary Alloys TDB v1
 PCHAT   =  Chatenay-Malabry Binary Alloys TDB v1
 PG35    =  G35 Binary Semi-Conductors TDB v1
 PION    =  TCS Public Ionic Solutions TDB v2
 PAQ2    =  TCS Public Aqueous Soln (SIT) TDB v2
 PAQS2   =  TCS Public Aqueous Soln (HKF) TDB v2
 PGEO    =  Saxena Pure Minerals Database v1
 MOB2    =  TCS Alloys Mobility Database v2
 MOB1    =  TCS Alloys Mobility Database v1
 MOBNI1  =  TCS Ni-Alloys Mobility Database v1
 MOBAL1  =  TCS Al-Alloys Mobility Database v1
 BISH    =  Bishop Dilute Al-Alloys MDB v1
 OIKA    =  Oikawa Dilute Fe-Alloys MDB v1
 PFRIB   =  Fridberg Dilute Fe-Alloys MDB v1
 USER    =  User defined Database

DATABASE NAME /TCFE6/: psub
 Current database: TCS Public Pure Substances TDB v1

 VA  DEFINED
TDB_PSUB: def-sys cu s o h
   ... the command in full is DEFINE_SYSTEM
 CU                     S                      O
 H  DEFINED
TDB_PSUB: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 GAS:G       :H H2 O O2 O3 H1O1 H1O2 H2O1 H2O2 S S2 S3 S4 S5 S6 S7 S8 O1S1
  O1S2 O2S1 O3S1 H1S1 H2S1 H2S2 H1O1S1_HSO H1O1S1_SOH H2O1S1_H2SO
  H2O1S1_HSOH H2O4S1 CU CU2 CU1H1 CU1O1 CU1H1O1 CU1S1 CU2S1:
  > Gaseous Mixture, using the ideal gas model
 CU          :CU:
  > This is pure Cu_FCC(A1)
 CU_L        :CU:
 S           :S:
  > This is pure S_FC_ORTHORHOMBIC
 S_S2        :S:
  > This is pure S_MONOCLINIC
 S_L         :S:
 H2O_L       :H2O1:
 H2O2_L      :H2O2:
 H2SO4_L     :H2O4S1:
 CUO         :CU1O1:
 CU2O        :CU2O1:
 CU2O_L      :CU2O1:
 CUS         :CU1S1:
 CU2S        :CU2S1:
 CU2S_S2     :CU2S1:
 CU2S_S3     :CU2S1:
 CU2S_L      :CU2S1:
 CUSO4       :CU1O4S1:
 CU2SO4      :CU2O4S1:
 CU2SO5      :CU2O5S1:
TDB_PSUB: @?<Hit_return_to_continue>
```

```
TDB_PSUB: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous species, stoichiometric solids and
      liquids in the Cu-Fe-H-N-O-S system.'
 -OK-
TDB_PSUB: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  EXIT                      REINITIATE_MODULE
 ADVANCED_OPTIONS         GOTO_MODULE               SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  HELP                      SELECT_EQUILIBRIUM
 BACK                     INFORMATION               SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_AXIS_VARIABLE        SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_CONDITIONS           SET_CONDITION
 COMPUTE_TRANSITION       LIST_EQUILIBRIUM          SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA   SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_STATUS               SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LIST_SYMBOLS              SET_REFERENCE_STATE
 DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM  SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN           SET_START_VALUE
 DELETE_SYMBOL            MAP                       SHOW_VALUE
 ENTER_SYMBOL             POST                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       READ_WORKSPACES           TABULATE
POLY_3: li-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 CU                       ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 S                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 S_S2                     ENTERED    0.00000000E+00  0.00000000E+00
 S_L                      ENTERED    0.00000000E+00  0.00000000E+00
 S                        ENTERED    0.00000000E+00  0.00000000E+00
 H2SO4_L                  ENTERED    0.00000000E+00  0.00000000E+00
 H2O_L                    ENTERED    0.00000000E+00  0.00000000E+00
 H2O2_L                   ENTERED    0.00000000E+00  0.00000000E+00
 CU_L                     ENTERED    0.00000000E+00  0.00000000E+00
 CUSO4                    ENTERED    0.00000000E+00  0.00000000E+00
 CUS                      ENTERED    0.00000000E+00  0.00000000E+00
 CUO                      ENTERED    0.00000000E+00  0.00000000E+00
 CU2S_S3                  ENTERED    0.00000000E+00  0.00000000E+00
 CU2S_S2                  ENTERED    0.00000000E+00  0.00000000E+00
 CU2S_L                   ENTERED    0.00000000E+00  0.00000000E+00
 CU2SO5                   ENTERED    0.00000000E+00  0.00000000E+00
 CU2SO4                   ENTERED    0.00000000E+00  0.00000000E+00
 CU2S                     ENTERED    0.00000000E+00  0.00000000E+00
 CU2O_L                   ENTERED    0.00000000E+00  0.00000000E+00
 CU2O                     ENTERED    0.00000000E+00  0.00000000E+00
 CU                       ENTERED    0.00000000E+00  0.00000000E+00
 GAS                      ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 CU          ENTERED    H15O10.5S1  ENTERED    O           ENTERED
 CU1H1       ENTERED    H1O1        ENTERED    O1S1        ENTERED
 CU1H10O9S1  ENTERED    H1O1S1_HSO  ENTERED    O1S2        ENTERED
 CU1H1O1     ENTERED    H1O1S1_SOH  ENTERED    O2          ENTERED
 CU1H2O2     ENTERED    H1O2        ENTERED    O2S1        ENTERED
 CU1H2O5S1   ENTERED    H1S1        ENTERED    O3          ENTERED
```

```
 CU1H6O7S1   ENTERED    H2          ENTERED    O3S1        ENTERED
 CU1O1       ENTERED    H2O1        ENTERED    S           ENTERED
 CU1O4S1     ENTERED    H2O1S1_H2SO ENTERED    S2          ENTERED
 CU1S1       ENTERED    H2O1S1_HSOH ENTERED    S3          ENTERED
 CU2         ENTERED    H2O2        ENTERED    S4          ENTERED
 CU2O1       ENTERED    H2O4S1      ENTERED    S5          ENTERED
 CU2O4S1     ENTERED    H2S1        ENTERED    S6          ENTERED
 CU2O5S1     ENTERED    H2S2        ENTERED    S7          ENTERED
 CU2S1       ENTERED    H4O5S1      ENTERED    S8          ENTERED
 H           ENTERED    H6O6S1      ENTERED    VA          ENTERED
 H10O8S1     ENTERED    H8O7S1      ENTERED
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Assume initially that we have one mole of Cu2S and 50 moles water vapor
POLY_3: s-i-a n(cu2s1)=1,n(h2o1)=50
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: set-cond t=1400,p=101325
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          685  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: PSUB

 Conditions:
 N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
 DEGREES OF FREEDOM 0

 Temperature   1400.00 K (  1126.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.53000E+02,  Mass in grams  1.05989E+03
 Total Gibbs energy -2.75931E+07,  Enthalpy -9.82382E+06,  Volume  5.76972E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CU                      2.0000E+00  1.1991E-01 1.6098E-03 -7.4867E+04 SER
 H                       1.0000E+02  9.5095E-02 9.5714E-06 -1.3452E+05 SER
 O                       5.0000E+01  7.5475E-01 5.1729E-11 -2.7570E+05 SER
 S                       1.0000E+00  3.0248E-02 2.0746E-08 -2.0593E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.5022E+02, Mass 9.0794E+02, Volume fraction 1.0000E+00  Mass fractions:
 O   8.81060E-01  H   1.11009E-01  S   7.92556E-03  CU  5.01241E-06
 Constitution:
 H2O1         9.86660E-01  CU1H1O1      1.96753E-08  CU1O1        8.58177E-12
 H2           8.86811E-03  O3S1         1.43507E-08  H2O2         5.46461E-12
 O2S1         4.44169E-03  H2O1S1_HSOH  7.52014E-09  H2O1S1_H2SO  3.12748E-12
 H2S1         2.10471E-05  S            4.30477E-09  H2O4S1       3.10120E-12
 O1S1         5.63051E-06  O2           2.46248E-09  S3           1.29650E-12
 CU           1.32327E-06  H1O1S1_SOH   1.77241E-09  H1O2         4.13438E-13
 H1O1         1.00104E-06  CU1S1        1.23642E-09  S4           3.25596E-18
 H            4.55656E-07  CU2          4.47851E-10  S5           1.21560E-21
 H1S1         3.40802E-07  CU2S1        2.11636E-10  O3           1.70006E-22
 S2           1.38936E-07  H2S2         1.77731E-10  S6           5.54892E-27
 CU1H1        8.04525E-08  O            4.66615E-11  S8           1.00000E-30
 O1S2         2.49875E-08  H1O1S1_HSO   3.35706E-11  S7           1.00000E-30

 CU2S_S3                     Status ENTERED     Driving force  0.0000E+00
 Moles 2.3266E+00, Mass 1.2343E+02, Volume fraction 0.0000E+00  Mass fractions:
 CU  7.98557E-01  S   2.01443E-01  O   0.00000E+00  H   0.00000E+00

 CU_L                        Status ENTERED     Driving force  0.0000E+00
 Moles 4.4883E-01, Mass 2.8522E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  1.00000E+00  S   0.00000E+00  O   0.00000E+00  H   0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Now set the status of the diginite (CU2S_S3) to be fixed with
```

```
POLY_3: @@ zero amount. This means that we will reduce this completely
POLY_3: c-s
   ... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): cu2s_s3
Status: /ENTERED/:  fix
Number of moles /0/:  0
POLY_3: @@ We have now too many conditions as we must allow the gas to vary
POLY_3: @@ in composition to find the correct oxygen potential
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
 FIXED PHASES
 CU2S_S3=0
 DEGREES OF FREEDOM -1
POLY_3: @?<Hit_return_to_continue>
POLY_3: set-c n(o)=none
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
 FIXED PHASES
 CU2S_S3=0
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          685  grid points in            1  s
    10 ITS,  CPU TIME USED   1 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: PSUB

 Conditions:
 N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
 FIXED PHASES
 CU2S_S3=0
 DEGREES OF FREEDOM 0

 Temperature   1400.00 K (  1126.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.54785E+02,  Mass in grams  1.08845E+03
 Total Gibbs energy -2.80759E+07,  Enthalpy -1.00131E+07,  Volume  5.85888E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CU                      2.0000E+00  1.1676E-01 1.6098E-03 -7.4867E+04 SER
 H                       1.0000E+02  9.2600E-02 6.5700E-06 -1.3890E+05 SER
 O                       5.1785E+01  7.6118E-01 1.0863E-10 -2.6707E+05 SER
 S                       1.0000E+00  2.9455E-02 2.0746E-08 -2.0593E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.5278E+02, Mass 9.6136E+02, Volume fraction 1.0000E+00  Mass fractions:
 O   8.61805E-01  H   1.04841E-01  S   3.33486E-02  CU  4.75131E-06
 Constitution:
 H2O1         9.76211E-01  O1S2         5.24705E-08  H2O4S1       2.84109E-11
 O2S1         1.95855E-02  CU1H1O1      2.83599E-08  CU1O1        1.80206E-11
 H2           4.17844E-03  O2           1.08582E-08  H2O2         1.13535E-11
 O1S1         1.18234E-05  H2O1S1_HSOH  7.44050E-09  H2O1S1_H2SO  3.09435E-12
 H2S1         9.91688E-06  S            4.30477E-09  S3           1.29650E-12
 H1O1         1.44290E-06  H1O1S1_SOH   2.55475E-09  H1O2         1.25138E-12
 CU           1.32327E-06  CU1S1        1.23642E-09  S4           3.25596E-18
 H            3.12773E-07  CU2          4.47851E-10  O3           1.57414E-21
 H1S1         2.33934E-07  CU2S1        2.11636E-10  S5           1.21560E-21
 S2           1.38936E-07  O            9.79832E-11  S6           5.54892E-27
 O3S1         1.32878E-07  H2S2         8.37427E-11  S8           1.00000E-30
 CU1H1        5.52244E-08  H1O1S1_HSO   4.83886E-11  S7           1.00000E-30

 CU_L                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00  Mass fractions:
 CU  1.00000E+00  S   0.00000E+00  O   0.00000E+00  H   0.00000E+00

 CU2S_S3                     Status FIXED       Driving force  0.0000E+00
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 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CU  7.98557E-01  S   2.01443E-01  O   0.00000E+00  H   0.00000E+00
POLY_3: sh n(*)
   ... the command in full is SHOW_VALUE
 N(CU)=2, N(H)=100., N(O)=51.784749, N(S)=1.
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ If we have too much oxygen we may get some copper oxides,
POLY_3: @@ check which one is the closest to be stable
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 CU2S_S3                FIXED      0.00000000E+00  0.00000000E+00
 CU_L                   ENTERED    0.00000000E+00  1.99992812E+00
 GAS                    ENTERED    0.00000000E+00  1.52784816E+02
 CU2S_L                 ENTERED   -3.93111389E-04  0.00000000E+00
 CU2S_S2                ENTERED   -3.30993574E-02  0.00000000E+00
 CU                     ENTERED   -3.54995984E-02  0.00000000E+00
 CU2S                   ENTERED   -3.33297445E-01  0.00000000E+00
 CU2O                   ENTERED   -1.08615273E+00  0.00000000E+00
 CU2O_L                 ENTERED   -1.23103598E+00  0.00000000E+00
 H2O_L                  ENTERED   -1.73886492E+00  0.00000000E+00
 CUS                    ENTERED   -3.17341693E+00  0.00000000E+00
 CUO                    ENTERED   -3.22972182E+00  0.00000000E+00
 CU2SO4                 ENTERED   -3.32220551E+00  0.00000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN -3.79759510E+00
 CU2SO5 CUSO4 H2SO4_L H2O2_L S_L S_S2 S
POLY_3: @@ Set Cu2O to fix with zero amount and remove the fix status of CU2S_S3
POLY_3: c-s p cu2o=fix 0
   ... the command in full is CHANGE_STATUS
POLY_3: c-s p cu2s_s3
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          685  grid points in            0  s
    39 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PSUB

 Conditions:
 N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
 FIXED PHASES
 CU2O=0
 DEGREES OF FREEDOM 0

 Temperature   1400.00 K (  1126.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.54993E+02,  Mass in grams  1.09178E+03
 Total Gibbs energy -2.81294E+07,  Enthalpy -1.00609E+07,  Volume  5.85900E+00

 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 CU                     2.0000E+00  1.1641E-01 1.6098E-03 -7.4867E+04 SER
 H                      1.0000E+02  9.2317E-02 1.2909E-06 -1.5784E+05 SER
 O                      5.1993E+01  7.6191E-01 2.8253E-09 -2.2914E+05 SER
 S                      1.0000E+00  2.9365E-02 3.0696E-11 -2.8178E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.5299E+02, Mass 9.6469E+02, Volume fraction 1.0000E+00  Mass fractions:
 O   8.62282E-01  H   1.04479E-01  S   3.32335E-02  CU  4.97350E-06
 Constitution:
 H2O1         9.80215E-01  H2O4S1       7.42671E-10  H1O1S1_HSO   3.65881E-13
 O2S1         1.96037E-02  H2S1         5.66454E-10  CU2S1        3.13135E-13
 H2           1.61310E-04  CU1O1        4.68706E-10  S2           3.04157E-13
 H1O1         7.37378E-06  CU2          4.47851E-10  H2O1S1_H2SO  4.59716E-15
 O2           7.34547E-06  H2O2         2.96508E-10  O3           2.76971E-17
 O3S1         3.45929E-06  H1O2         1.66331E-10  H2S2         7.07748E-18
 CU           1.32327E-06  H1S1         6.80080E-11  S3           4.19951E-21
 O1S1         4.55002E-07  H1O1S1_SOH   1.93172E-11  S4           1.56044E-29
 CU1H1O1      1.44930E-07  H2O1S1_HSOH  1.10541E-11  S7           1.00000E-30
 H            6.14543E-08  S            6.36932E-12  S5           1.00000E-30
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 CU1H1        1.08506E-08  O1S2         2.98765E-12  S6           1.00000E-30
 O            2.54848E-09  CU1S1        1.82939E-12  S8           1.00000E-30

 CU_L                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00  Mass fractions:
 CU  1.00000E+00  S   0.00000E+00  O   0.00000E+00  H   0.00000E+00

 CU2O                       Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CU  8.88190E-01  O   1.11810E-01  S   0.00000E+00  H   0.00000E+00
POLY_3: show n(*)
   ... the command in full is SHOW_VALUE
 N(CU)=2, N(H)=100., N(O)=51.992866, N(S)=1.
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The ratio N(O) to N(H) should thus be between 0.5178 and 0.52
POLY_3: @@ in order to reduce all Cu2S and not forming any Cu2O
POLY_3: @@ Make a diagram showing this amounts of phases
POLY_3: c-st p cu2o
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: s-a-v 1 n(o)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  45
Max value /1/:  55
Increment /.25/:
POLY_3: s-c n(o)
   ... the command in full is SET_CONDITION
Value /51.99286556/:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          685  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex11 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    51.9929
 Global calculation of initial equilibrium ....OK

 Phase Region from    51.9929     for:
     GAS
     CU_L
 Global check of adding phase at  5.19929E+01
 Calculated     2 equilibria

 Phase Region from    51.9929     for:
     GAS
     CU2O
     CU_L
 Global check of removing phase at  5.29928E+01
 Calculated     6 equilibria

 Phase Region from    52.9928     for:
     GAS
     CU2O
 Global test at  5.49929E+01 .... OK
 Terminating at    55.0000
 Calculated    12 equilibria

 Phase Region from    51.9929     for:
     GAS
     CU_L
 Global check of adding phase at  5.17847E+01
 Calculated     3 equilibria

 Phase Region from    51.7847     for:
     GAS
     CU2S_S3
     CU_L
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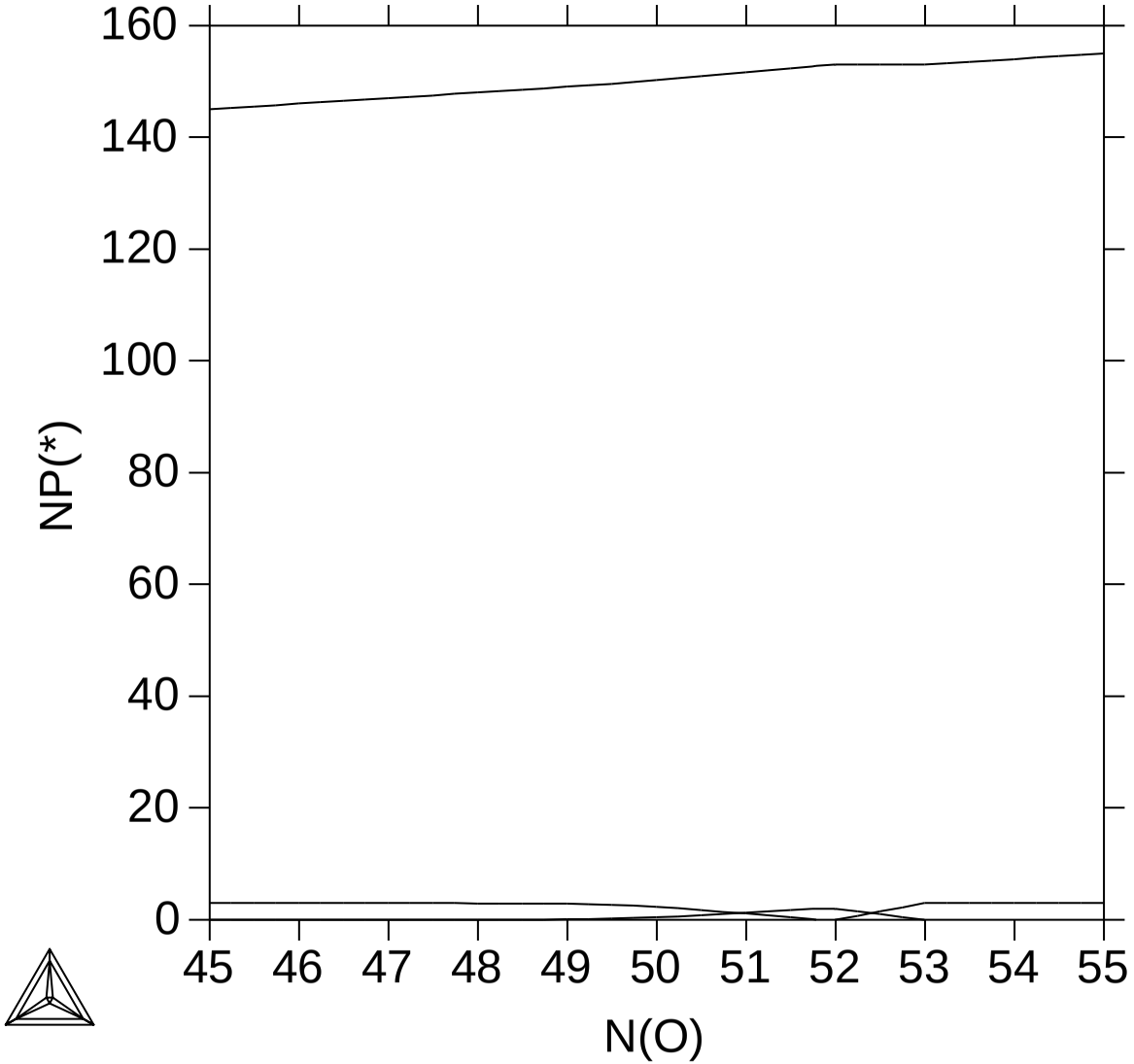
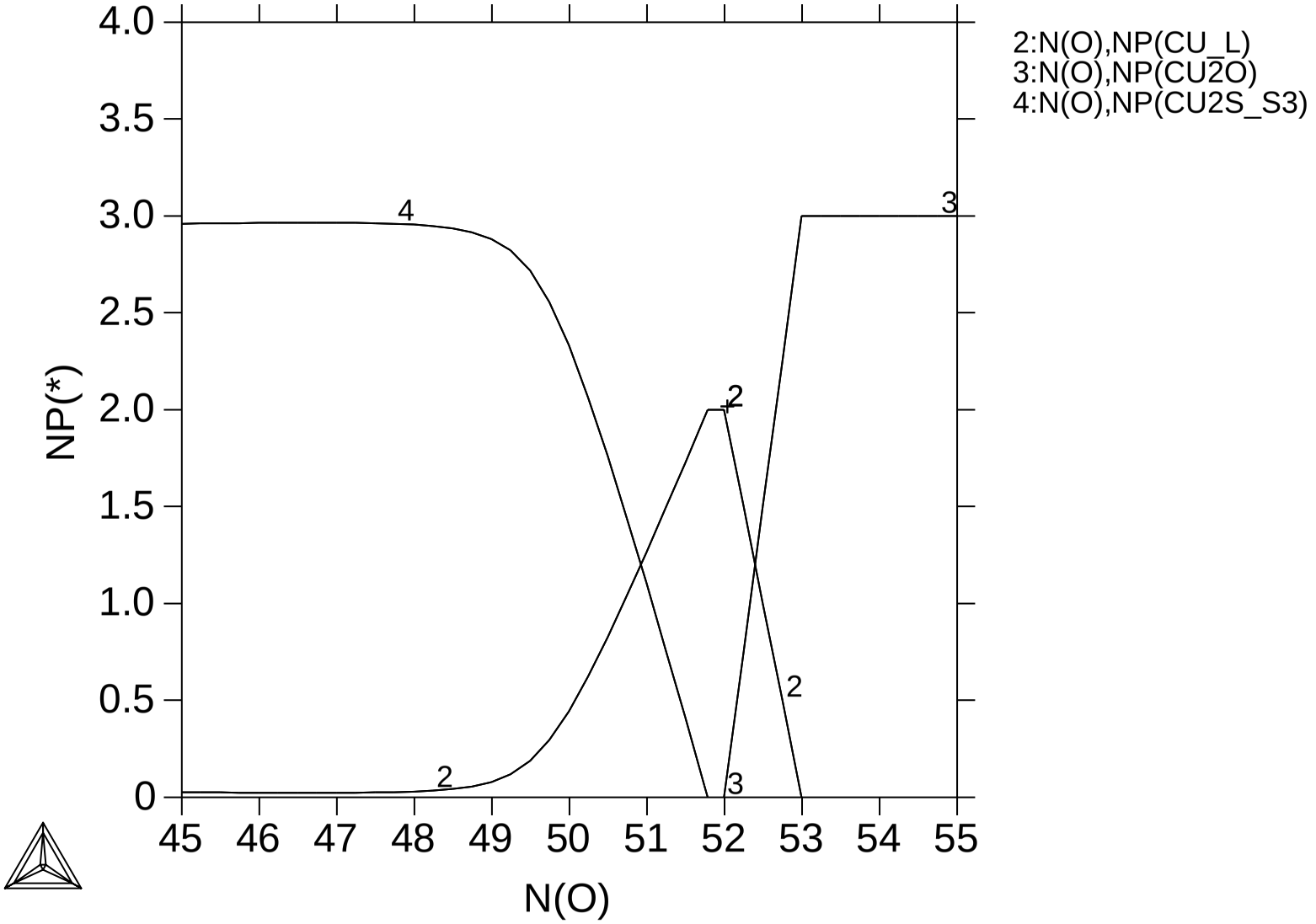
 Global test at  4.99929E+01 .... OK
 Global test at  4.74929E+01 .... OK
 Global test at  4.50000E+01 .... OK
 Terminating at    45.0000
 Calculated    31 equilibria
 *** Buffer saved on file: tcex11.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-d-a x n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 11a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s y n 0 4
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 11b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           1  seconds
```

THERMO-CALC (2009.04.15:03.02) :example 11a
DATABASE:PSUB
N(CU)=2, N(S)=1., N(H)=100., T=1400, P=1.01325E5;



THERMO-CALC (2009.04.15:03.02) :example 11b
DATABASE:PSUB
N(CU)=2, N(S)=1., N(H)=100., T=1400, P=1.01325E5;



12

Tabulation of thermodynamic data for reactions

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ This example shows a number of independent cases using the
SYS: @@ tabulation module. This module is very rudimentary but still
SYS: @@ provides some facilities. Note that there is no on-line help available!
SYS: @@ Each case is separated by a line of ============================
SYS: set-log ex12,,
SYS: go tab
   ... the command in full is GOTO_MODULE
TAB: ?
   ... the command in full is HELP
 BACK                    LIST_SUBSTANCES          SWITCH_DATABASE
 ENTER_FUNCTION          MACRO_FILE_OPEN          TABULATE_DERIVATIVES
 ENTER_REACTION          PATCH                    TABULATE_REACTION
 EXIT                    SET_ENERGY_UNIT          TABULATE_SUBSTANCE
 GOTO_MODULE             SET_INTERACTIVE
TAB: @@ Tabulate data for a reaction
TAB: tab-rea 3H2+N2=2N1H3;
   ... the command in full is TABULATE_REACTION
 Use one of these databases

 TCFE6   =  TCS Steels/Fe-Alloys Database v6
 TCFE5   =  TCS Steels/Fe-Alloys Database v5
 TCFE4   =  TCS Steels/Fe-Alloys Database v4
 TCFE3   =  TCS Steels/Fe-Alloys Database v3
 TCFE2   =  TCS Steels/Fe-Alloys Database v2
 TCFE1   =  TCS Steels/Fe-Alloys Database v1
 FEDAT   =  TCS/TT Steels Database v1
 TCNI1   =  TCS Ni-Alloys Database v1
 SSOL4   =  SGTE Alloy Solutions Database v4
 SSOL2   =  SGTE Alloy Solutions Database v2
 SBIN2   =  SGTE Binary Alloys Database v2
 SSUB4   =  SGTE Substances Database v4
 SPOT4   =  SGTE Potential Database v4
 SSUB3   =  SGTE Substances Database v3
 SPOT3   =  SGTE Potential Database v3
 SSUB2   =  SGTE Substances Database v2
 SPOT2   =  SGTE Potential Database v2
 SNOB1   =  SGTE Nobel Metal Alloys Database v2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1
 SALT1   =  SGTE Molten Salt Database v1
 SNUX6   =  SGTE In-Vessel Nuclear Oxide TDB v6.2
 SEMC2   =  TC Semi-Conductors Database v2
 SLAG2   =  TCS Fe-containing Slag Database v2
 SLAG1   =  TCS Fe-containing Slag Database v1
 ION2    =  TCS Ionic Solutions Database v2
 ION1    =  TCS Ionic Solutions Database v1
 NOX2    =  NPL Oxide Solutions Database, v2
 NSLD2   =  NPL Solder Alloys Database v2
 TCMP2   =  TCS Materials Processing Database v2
 TCES1   =  TCS Combustion/Sintering Database v1
 NUMT2   =  TCS Nuclear Materials Database v2
 NUOX4   =  TCS Nuclear Oxides Database v4
 NUTO1   =  TCS U-Zr-Si Ternary Oxides TDB v1
 NUTA1   =  TCS Ag-Cd-In Ternary Alloys TDB v1
 TCNF2   =  TCS Nuclear Fuels Database v2
 TTNI7   =  TT Ni-Alloys Database v7
 TTNI6   =  TT Ni-Alloys Database v6
 TTNI5   =  TT Ni-Alloys Database v5
 TTNF5   =  TT NiFe-Alloys Database v5
 TTTI3   =  TT Ti-Alloys Database v3
 TTTI2   =  TT Ti-Alloys Database v2
 TTTIAL  =  TT TiAl-Alloys Database v1
 TTAL6   =  TT Al-Alloys Database v6
 TTAL5   =  TT Al-Alloys Database v5
 TTAL4   =  TT Al-Alloys Database v4
 TTAL3   =  TTAL3setup.TDC TT Al-Alloys Database v3
```

```
 TTMG4   =  TT Mg-Alloys Database v4
 TTMG3   =  TT Mg-Alloys Database v3
 TTMG2   =  TT Mg-Alloys Database v2
 TTZR1   =  TT Zr-Alloys Database v1
 TCAQ2   =  TCS Aqueous Solution Database v2
 AQS2    =  TGG Aqueous Solution Database v2
 GCE2    =  TGG Geochemical/Environmental TDB v2
 CCC1    =  CCT Cemented Carbides Database v1
 PURE4   =  SGTE Unary (Pure Elements) TDB v4
 PSUB    =  TCS Public Pure Substances TDB v1
 PBIN    =  TCS Public Binary Alloys TDB v1
 PTERN   =  TCS Public Ternary Alloys TDB v1
 PKP     =  Kaufman Binary Alloys TDB v1
 PCHAT   =  Chatenay-Malabry Binary Alloys TDB v1
 PG35    =  G35 Binary Semi-Conductors TDB v1
 PION    =  TCS Public Ionic Solutions TDB v2
 PAQ2    =  TCS Public Aqueous Soln (SIT) TDB v2
 PAQS2   =  TCS Public Aqueous Soln (HKF) TDB v2
 PGEO    =  Saxena Pure Minerals Database v1
 MOB2    =  TCS Alloys Mobility Database v2
 MOB1    =  TCS Alloys Mobility Database v1
 MOBNI1  =  TCS Ni-Alloys Mobility Database v1
 MOBAL1  =  TCS Al-Alloys Mobility Database v1
 BISH    =  Bishop Dilute Al-Alloys MDB v1
 OIKA    =  Oikawa Dilute Fe-Alloys MDB v1
 PFRIB   =  Fridberg Dilute Fe-Alloys MDB v1
 USER    =  User defined Database

DATABASE NAME /TCFE6/: SSUB3
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: SGTE Substances Database v3

 VA  DEFINED
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 H2                    N2                    H3N1
   DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      HYDROGEN<G>
      STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   H3N1<G> T.C.R.A.S. Class: 2
      AMMONIA <GAS>
   N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      NITROGEN <DIATOMIC GAS>
      PUBLISHED BY JANAF AT 09/65
 -OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100
Output file /SCREEN/:

              O U T P U T  F R O M  T H E R M O - C A L C
              2009. 4.15                          3. 2.14

 Reaction:  3H2<G>+N2<G>=2H3N1<G>
 H2<GAS>
 N2<GAS>
 H3N1<GAS>

 ****************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G
  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
```

```
 ********************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04
  800.00  -1.81081E+01  -1.07390E+05  -2.30808E+02   7.72568E+04
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05
 1100.00  -7.77554E+00  -1.11169E+05  -2.34908E+02   1.47229E+05
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05
TAB: @?<Hit_return_to_continue>
TAB: @@ Add a final column with a function. In this function
TAB: @@ you may use G, S, H, V, CP, T and R with their obvious
TAB: @@ meaning. You may also use H298 and ALPHA (thermal expansivity)
TAB: @@ and KAPPA (isothermal compressibility). In most databases
TAB: @@ there are no pressure dependence and thus V, ALPHA and KAPPA
TAB: @@ will not be correct.
TAB: e-fun
   ... the command in full is ENTER_FUNCTION
Name: fef
Function: (g-h298)/t
&
TAB: t-r
   ... the command in full is TABULATE_REACTION
Same reaction? /Y/:  y
Pressure /100000/:  100000
Low temperature limit /298.15/:  298.15
High temperature limit /2000/:  2000
Step in temperature /100/:  100
Output file /SCREEN/:

              O U T P U T   F R O M   T H E R M O - C A L C
              2009. 4.15                          3. 2.14

 Column 6: fef       (G-H298 )/T
 Reaction:  3H2<G>+N2<G>=2H3N1<G>
 H2<GAS>
 N2<GAS>
 H3N1<GAS>

 ********************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ********************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04   1.98115E+02
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04   1.98116E+02
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04   1.99799E+02
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03   2.02800E+02
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04   2.05930E+02
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04   2.08834E+02
  800.00  -1.81081E+01  -1.07390E+05  -2.30808E+02   7.72568E+04   2.11421E+02
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05   2.13687E+02
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05   2.15659E+02
 1100.00  -7.77554E+00  -1.11169E+05  -2.34908E+02   1.47229E+05   2.17372E+02
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05   2.18858E+02
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05   2.20149E+02
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05   2.21272E+02
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05   2.22251E+02
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05   2.23107E+02
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05   2.23857E+02
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05   2.24515E+02
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05   2.25093E+02
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05   2.25602E+02
TAB: @?<Hit_return_to_continue>
```

```
TAB: t-r
   ... the command in full is TABULATE_REACTION
Same reaction? /Y/:  y
Pressure /100000/:  100000
Low temperature limit /298.15/:  298.15
High temperature limit /2000/:  2000
Step in temperature /100/:  100
Output file /SCREEN/:  tcex12a
Grapical output? /Y/:  y
Plot column? /2/:  6
              O U T P U T  F R O M  T H E R M O - C A L C
              2009. 4.15                          3. 2.14

 Column 6: fef       (G-H298 )/T
 Reaction:  3H2<G>+N2<G>=2H3N1<G>
 H2<GAS>
 N2<GAS>
 H3N1<GAS>

 ********************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ********************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04   1.98115E+02
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04   1.98116E+02
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04   1.99799E+02
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03   2.02800E+02
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04   2.05930E+02
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04   2.08834E+02
  800.00  -1.81081E+01  -1.07390E+05  -2.30808E+02   7.72568E+04   2.11421E+02
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05   2.13687E+02
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05   2.15659E+02
 1100.00  -7.77554E+00  -1.11169E+05  -2.34908E+02   1.47229E+05   2.17372E+02
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05   2.18858E+02
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05   2.20149E+02
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05   2.21272E+02
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05   2.22251E+02
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05   2.23107E+02
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05   2.23857E+02
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05   2.24515E+02
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05   2.25093E+02
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05   2.25602E+02

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is SET_SCALING_STATUS
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-title example 12a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: back
TAB:
TAB:
TAB: @@ In the Gibbs-Enery-System we can list the data we use
TAB: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: l-d
   ... the command in full is LIST_DATA
OUTPUT FILE: /SCREEN/:
OPTIONS?: ?
 OPTIONS?

  Choose one or several of the following options for output:
   * N  the output is written as a ''user'' database format.
   * P  the output is written as a MACRO file for future input.
          This is useful for creating setup files for assessments.
   * S  the symbols are suppressed.
```

```
   * R  the references for the parameters are listed
          (only for some databases in which references are available)
   * L  the output is written suitable for a LaTeX preprocessor.

OPTIONS?: rs
1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH          DATE 2009- 4-15
 FROM DATABASE: SSUB3

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 H    1/2_MOLE_H2(GAS)          1.0079E+00  4.2340E+03  6.5285E+01
  2 N    1/2_MOLE_N2(GAS)          1.4007E+01  4.3350E+03  9.5751E+01

 SPECIES                                  STOICHIOMETRY
   1 H                                    H
   2 H2                                   H2
   3 H3N1                                 H3N1
   4 N                                    N
   5 N2                                   N2
   6 VA                                   VA

 GAS
    CONSTITUENTS: H2,H3N1,N2

      G(GAS,H2;0)- 2 H298(1/2_MOLE_H2(GAS),H;0) = +F10854T+R*T*LN(1E-05*P)
           REFERENCE: 6138
      G(GAS,H3N1;0)- 3 H298(1/2_MOLE_H2(GAS),H;0)-H298(1/2_MOLE_N2(GAS),N;0)
           = +F11101T+R*T*LN(1E-05*P)
           REFERENCE: 6263
      G(GAS,N2;0)- 2 H298(1/2_MOLE_N2(GAS),N;0) = +F12981T+R*T*LN(1E-05*P)
           REFERENCE: 7357

 LIST_OF_REFERENCES
 NUMBER  SOURCE
   REF6138 H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
         HYDROGEN<G>
         STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   REF6263 H3N1<G> T.C.R.A.S. Class: 2
         AMMONIA <GAS>
   REF7357 N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
         NITROGEN <DIATOMIC GAS>
         PUBLISHED BY JANAF AT 09/65

GES: @?<Hit_return_to_continue>
GES: back
TAB:
TAB: @@ Tabulate another reaction ==============================================
TAB: t-r
   ... the command in full is TABULATE_REACTION
Same reaction? /Y/:  n
Reaction: INP+GA=GAP+IN;
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 GA                    IN1P1                  IN
 GA1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   GA1<G> T.C.R.A.S. Class: 1
      GALLIUM <GAS>
   GA1P1<G> S.G.T.E.
      GALLIUM PHOSPHIDE <GAS>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
```

```
      from T.C.R.A.S.
   IN1<G> T.C.R.A.S. Class: 1
   IN1P1<G> CHATILLON(1994 March)
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   GA1P1 S.G.T.E.
      GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
   GA1 S.G.T.E. **
      GALLIUM
      Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
   IN1P1 I. BARIN 3rd. Edition
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
   IN1 S.G.T.E. **
      INDIUM
      Data from SGTE Unary DB
 -OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100
Output file /tcex12a/: tcex12b
Grapical output? /Y/: Y
Plot column? /2/: 2
              O U T P U T  F R O M  T H E R M O - C A L C
              2009. 4.15                          3. 2.15

 Column 6: fef       (G-H298 )/T
 Reaction:  GA+IN1P1=IN+GA1P1
 GA stable as GA_S
 IN1P1 stable as IN1P1_S
 IN stable as IN_S
 GA1P1 stable as GA1P1_S

 ********************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ********************************************************************************
  298.15  -1.56785E+00  -4.01610E+04   4.46600E+00  -4.14925E+04  -4.46600E+00
  300.00  -1.60915E+00  -4.01639E+04   4.45617E+00  -4.15008E+04  -4.46597E+00
  302.   ---- GA becomes GA_L ,delta-H =   5589.80
  400.00  -6.09329E-01  -4.59820E+04  -1.46756E+01  -4.01118E+04   1.23002E-01
  430.   ---- IN becomes IN_L ,delta-H =   3283.00
  500.00   7.26020E-01  -4.26605E+04  -6.95385E+00  -3.91835E+04   1.95492E+00
  600.00   1.12393E+00  -4.25671E+04  -6.78469E+00  -3.84963E+04   2.77457E+00
  700.00   1.32655E+00  -4.24423E+04  -6.59282E+00  -3.78274E+04   3.33376E+00
  800.00   1.22407E+00  -4.23120E+04  -6.41862E+00  -3.71771E+04   3.72988E+00
  900.00   7.64029E-01  -4.22095E+04  -6.29733E+00  -3.65419E+04   4.02125E+00
 1000.00  -8.12013E-02  -4.21720E+04  -6.25712E+00  -3.59149E+04   4.24608E+00
 1100.00  -1.32730E+00  -4.22391E+04  -6.32007E+00  -3.52870E+04   4.43091E+00
 1200.00  -2.98369E+00  -4.24512E+04  -6.50358E+00  -3.46469E+04   4.59509E+00
 1300.00  -5.05634E+00  -4.28497E+04  -6.82145E+00  -3.39818E+04   4.75323E+00
 Temperature range exceeded for IN1P1

   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is SET_SCALING_STATUS
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-title example 12b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: back
TAB:
TAB:
TAB: @@ By default a species in a gas is not included in
TAB: @@ a tabulation, you must specify <GAS> if you want that
TAB: t-r n
   ... the command in full is TABULATE_REACTION
Reaction: INP<gas>+GA=GAP+IN;
   ... the command in full is REJECT
```

```
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 GA                    IN1P1                   IN
 GA1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   GA1<G> T.C.R.A.S. Class: 1
      GALLIUM <GAS>
   GA1P1<G> S.G.T.E.
      GALLIUM PHOSPHIDE <GAS>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
      from T.C.R.A.S.
   IN1<G> T.C.R.A.S. Class: 1
   IN1P1<G> CHATILLON(1994 March)
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   GA1P1 S.G.T.E.
      GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
   GA1 S.G.T.E. **
      GALLIUM
      Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
   IN1P1 I. BARIN 3rd. Edition
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
   IN1 S.G.T.E. **
      INDIUM
      Data from SGTE Unary DB
 -OK-
Pressure /100000/:  100000
Low temperature limit /298.15/:  1000
High temperature limit /2000/:  2000
Step in temperature /100/:  100
Output file /tcex12b/:
Grapical output? /Y/:  N
               O U T P U T  F R O M  T H E R M O - C A L C
               2009. 4.15                          3. 2.15

 Column 6: fef       (G-H298 )/T
 Reaction:  GA+IN1P1<G>=IN+GA1P1
 GA stable as GA_L
 IN1P1<GAS>
 IN1P1<GAS>
 IN stable as IN_L
 GA1P1 stable as GA1P1_S

 ********************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ********************************************************************************
 1000.00   1.57503E+01  -4.65760E+05  -1.78780E+02  -2.86980E+05   1.86368E+02
 1000.00   1.57503E+01  -4.65760E+05  -1.78780E+02  -2.86980E+05   1.86368E+02
 1100.00   1.60263E+01  -4.64172E+05  -1.77266E+02  -2.69179E+05   1.85608E+02
 1100.00   1.60263E+01  -4.64172E+05  -1.77266E+02  -2.69179E+05   1.85608E+02
 1200.00   1.63030E+01  -4.62555E+05  -1.75860E+02  -2.51523E+05   1.84854E+02
 1200.00   1.63030E+01  -4.62555E+05  -1.75860E+02  -2.51523E+05   1.84854E+02
 1300.00   1.65828E+01  -4.60911E+05  -1.74544E+02  -2.34004E+05   1.84111E+02
 1300.00   1.65828E+01  -4.60911E+05  -1.74544E+02  -2.34004E+05   1.84111E+02
 1400.00   1.68674E+01  -4.59238E+05  -1.73305E+02  -2.16612E+05   1.83383E+02
 1400.00   1.68674E+01  -4.59238E+05  -1.73305E+02  -2.16612E+05   1.83383E+02
 1500.00   1.71578E+01  -4.57537E+05  -1.72131E+02  -1.99341E+05   1.82672E+02
 1500.00   1.71578E+01  -4.57537E+05  -1.72131E+02  -1.99341E+05   1.82672E+02
 1600.00   1.74548E+01  -4.55807E+05  -1.71014E+02  -1.82184E+05   1.81978E+02
 1600.00   1.74548E+01  -4.55807E+05  -1.71014E+02  -1.82184E+05   1.81978E+02
 1700.00   1.77590E+01  -4.54046E+05  -1.69947E+02  -1.65136E+05   1.81301E+02
 1700.00   1.77590E+01  -4.54046E+05  -1.69947E+02  -1.65136E+05   1.81301E+02
 Temperature range exceeded for GA1P1
```

TAB: **@?<Hit_return_to_continue>**
TAB: *@@* **==========**
TAB: *@@ You can list substances in the database*
TAB: **li-sub**
... the command in full is LIST_SUBSTANCES
... the command in full is REJECT
VA DEFINED
REINITIATING GES5 .....
... the command in full is DEFINE_SPECIES
AG DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES ......
PHASES ....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

AG1<G> T.C.R.A.S. Class: 1
SILVER <GAS>
AG1 HULTGREN SELECTED VAL. SGTE **
SILVER
CODATA KEY VALUE.MPT=1234.93K.
--U.D. 30/10/85 .
-OK-
With elements /*/: **IN P**
Exclusivly with those elements? /Y/:

IN	P	IN2
IN1P1	P2	P3
P4		

TAB: *@@ or all substances with Fe*
TAB: **li-sub**
... the command in full is LIST_SUBSTANCES
With elements /*/: **FE**
Exclusivly with those elements? /Y/: **N**

FE	AL2FE1O4	AS1FE1O4
AS2FE3O8	B1FE1	B1FE2
BR1FE1	BR2FE1	BR3FE1
BR4FE2	BR6FE2	C1FE1O3
C1FE3	C5FE1O5	CA1FE2O4
CA2FE2O5	CD1FE2O4	CL1FE1
CL1FE1O1	CL2FE1	CL3FE1
CL4FE2	CL6FE2	CO1FE2O4
CR2FE1O4	CU1FE1O2	CU1FE1S2
CU1FE2O4	CU2FE2O4	CU5FE1S4
F1FE1	F2FE1	F3FE1
F4FE2	F6FE2	FE1/+1
FE1/-1	FE2	FE1H1
FE1H1O1	FE1H1O2	FE1H2O2
FE1H3O3	FE1H4O6P1	FE1I1
FE1I2	FE1I3	FE1K1O2
FE1K2O2	FE1K4O3	FE1LI1O2
FE1LI5O4	FE1MO1O4	FE1NA1O2
FE.877S1	FE.947O1	FE1O1
FE1O2	FE1O3SI1	FE1O3TI1
FE1O4S1	FE1O4V2	FE1O4W1
FE1O6V2	FE1P1	FE1P2
FE1S1	FE1S2	FE1SE.966
FE1SE1	FE1SI1	FE1SI2
FE1SI2.33	FE1TE.99	FE1TE1
FE1TE2	FE1TI1	FE2H2O4
FE2I4	FE2I6	FE2LI2O4
FE2MG1O4	FE2MN1O4	FE2N1
FE2NB1	FE2NI1O4	FE2O12S3
FE2O3	FE2O4SI1	FE2O4TI1
FE2O4ZN1	FE2P1	FE2TA1
FE2TI1	FE2U1	FE3LI2O5
FE3MO2	FE3O4	FE3P1
FE3W2	FE4N1	FE5LI1O8

TAB:
TAB: **@?<Hit_return_to_continue>**
TAB: *@@* **==========**
TAB: *@@ You can tabulate data for a substance or phase also, this is equivalent*

```
TAB: @@ with tabels you may find in JANAF for example
TAB: t-sub IN1P1
   ... the command in full is TABULATE_SUBSTANCE
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 IN1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   IN1P1<G> CHATILLON(1994 March)
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   IN1P1 I. BARIN 3rd. Edition
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
 -OK-
Pressure /100000/:  100000
Low temperature limit /1000/:  300
High temperature limit /2000/:  1300
Step in temperature /100/:  100
Output file /tcex12b/:  tcex12c
Grapical output? /Y/:  Y
Plot column? /2/:  2
              O U T P U T  F R O M  T H E R M O - C A L C
              2009. 4.15                          3. 2.15

 Column 6: fef       (G-H298 )/T

 Phase : IN1P1_S                   Pressure :      100000.00
 Specie: IN1P1

 ********************************************************************************
    T      Cp            H             S             G            fef
  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ********************************************************************************
  300.00   4.62734E+01  -7.44015E+04   6.42060E+01  -9.36633E+04  -6.39209E+01
  400.00   4.89412E+01  -6.96137E+04   7.79614E+01  -1.00798E+05  -6.57782E+01
  500.00   4.97376E+01  -6.46723E+04   8.89845E+01  -1.09165E+05  -6.93552E+01
  600.00   5.00615E+01  -5.96811E+04   9.80837E+01  -1.18531E+05  -7.34072E+01
  700.00   5.03923E+01  -5.46595E+04   1.05824E+02  -1.28736E+05  -7.74989E+01
  800.00   5.09302E+01  -4.95956E+04   1.12585E+02  -1.39664E+05  -8.14708E+01
  900.00   5.17709E+01  -4.44633E+04   1.18629E+02  -1.51229E+05  -8.52694E+01
 1000.00   5.29647E+01  -3.92297E+04   1.24142E+02  -1.63372E+05  -8.88848E+01
 1100.00   5.45403E+01  -3.38577E+04   1.29261E+02  -1.76045E+05  -9.23252E+01
 1200.00   5.65148E+01  -2.83083E+04   1.34088E+02  -1.89214E+05  -9.56061E+01
 1300.00   5.88991E+01  -2.25410E+04   1.38703E+02  -2.02855E+05  -9.87449E+01
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST: @?<Hit_return_to_continue>
POST:
POST: set-title example 12c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: back
TAB: @@ ============================================================================
TAB: @@ In order to obtain the partial pressure of a species in
TAB: @@ the gas in its pure condenced state you can enter a reaction
TAB: @@ like this for KOH. The partial pressure is entered as a
TAB: @@ function exp(-G/R/T)
TAB: e-fun
   ... the command in full is ENTER_FUNCTION
Name: pp
```

```
Function: exp(-g/r/t);
TAB:
TAB: tab-r n K1O1H1=K1H1O1<g>
   ... the command in full is TABULATE_REACTION
&
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_SPECIES
 H1K1O1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   H1K1O1<G> J. Phys. Chem. Ref. Data
      Data taken from JPCRD, 26, 4 1031-1110 (1997)
   H1K1O1 J. Phys. Chem. Ref. Data
      Data taken from JPCRD, 26, 4 1031-1110 (1997)
 -OK-
Pressure /100000/:  100000
Low temperature limit /300/:  300
High temperature limit /1300/:  2000
Step in temperature /100/:  100
Output file /tcex12c/:  tcex12d
Grapical output? /Y/:  Y
Plot column? /2/:  6
              O U T P U T  F R O M  T H E R M O - C A L C
              2009. 4.15                          3. 2.15

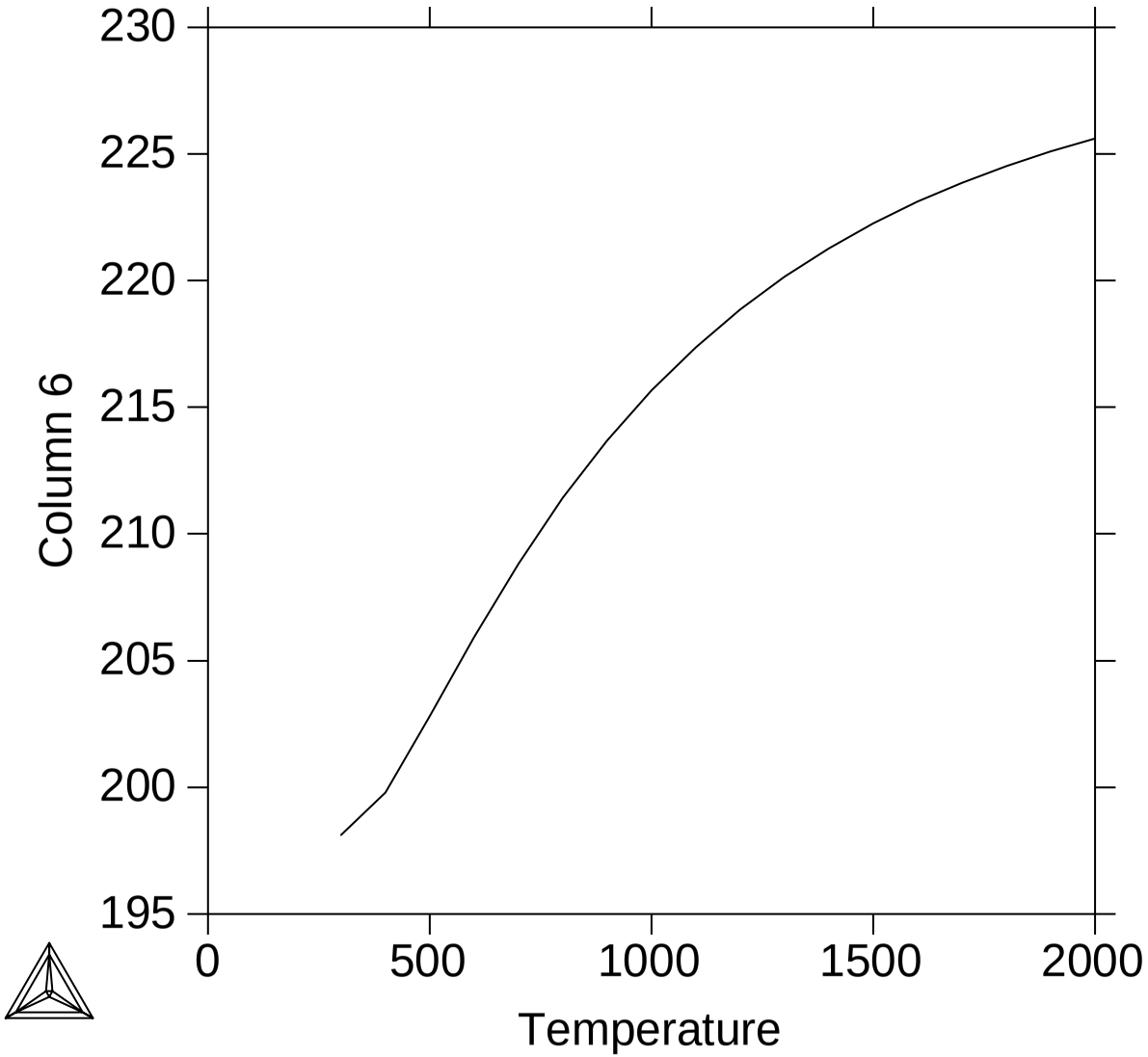
 Column 6: pp        EXP(-G/R/T )
 Reaction:  H1K1O1=H1K1O1<G>
 H1K1O1 stable as H1K1O1_S
 H1K1O1<GAS>

 ********************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       pp
  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ********************************************************************************
  300.00  -1.97899E+01   1.92543E+05   1.56915E+02   1.45469E+05   4.70147E-26
  400.00  -2.31294E+01   1.90409E+05   1.50797E+02   1.30090E+05   1.02900E-17
  500.00  -2.73216E+01   1.87890E+05   1.45195E+02   1.15293E+05   9.03075E-13
  517.   ---- H1K1O1 becomes H1K1O1_S2 ,delta-H =   5600.00
  600.00  -2.71797E+01   1.79542E+05   1.29351E+02   1.01932E+05   1.33747E-09
  680.   ---- H1K1O1 becomes H1K1O1_L ,delta-H =   7900.00
  700.00  -3.36564E+01   1.68804E+05   1.13354E+02   8.94566E+04   2.11269E-07
  800.00  -3.31914E+01   1.65462E+05   1.08890E+02   7.83499E+04   7.66317E-06
  900.00  -3.27453E+01   1.62165E+05   1.05007E+02   6.76592E+04   1.18375E-04
 1000.00  -3.22973E+01   1.58913E+05   1.01580E+02   5.73333E+04   1.01226E-03
 1100.00  -3.18358E+01   1.55706E+05   9.85231E+01   4.73310E+04   5.65583E-03
 1200.00  -3.13536E+01   1.52547E+05   9.57735E+01   3.76185E+04   2.30437E-02
 1300.00  -3.08463E+01   1.49436E+05   9.32837E+01   2.81676E+04   7.38312E-02
 1400.00  -3.03294E+01   1.46378E+05   9.10171E+01   1.89543E+04   1.96257E-01
 1500.00  -2.98854E+01   1.43368E+05   8.89402E+01   9.95788E+03   4.50033E-01
 1600.00  -2.94990E+01   1.40399E+05   8.70240E+01   1.16091E+03   9.16434E-01
 1700.00  -2.91580E+01   1.37467E+05   8.52461E+01  -7.45152E+03   1.69415E+00
 1800.00  -2.88535E+01   1.34567E+05   8.35882E+01  -1.58923E+04   2.89182E+00
 1900.00  -2.85787E+01   1.31695E+05   8.20357E+01  -2.41727E+04   4.61888E+00
 2000.00  -2.83287E+01   1.28850E+05   8.05762E+01  -3.23025E+04   6.97645E+00

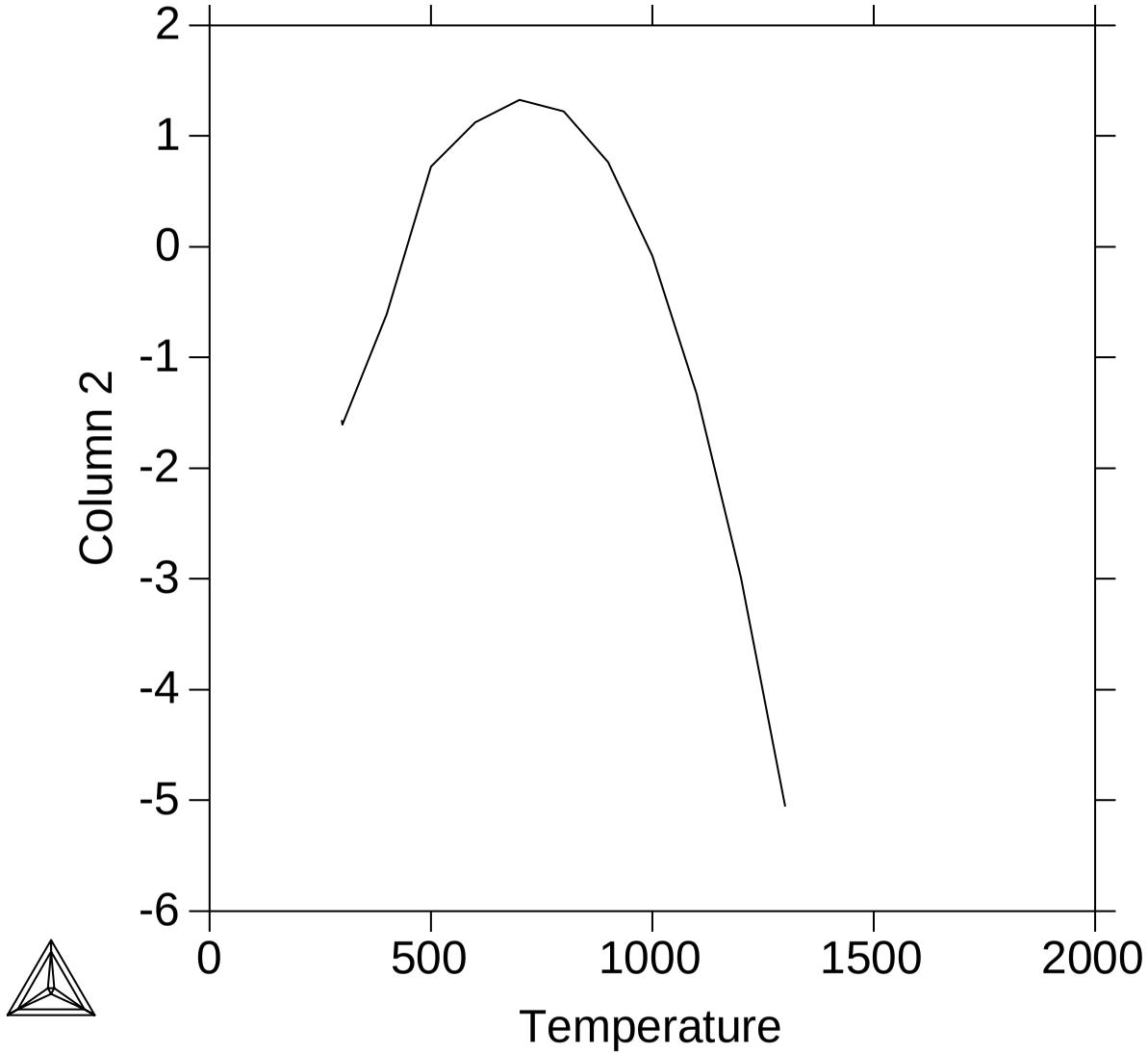
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is SET_SCALING_STATUS
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-title example 12d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
```

POST: **@?<Hit_return_to_continue>**
POST: **s-a-ty y**
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: **log**
POST: **set-title example 12e**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **back**
TAB: **set-inter**
   ... the command in full is SET_INTERACTIVE
TAB: CPU time   2 seconds

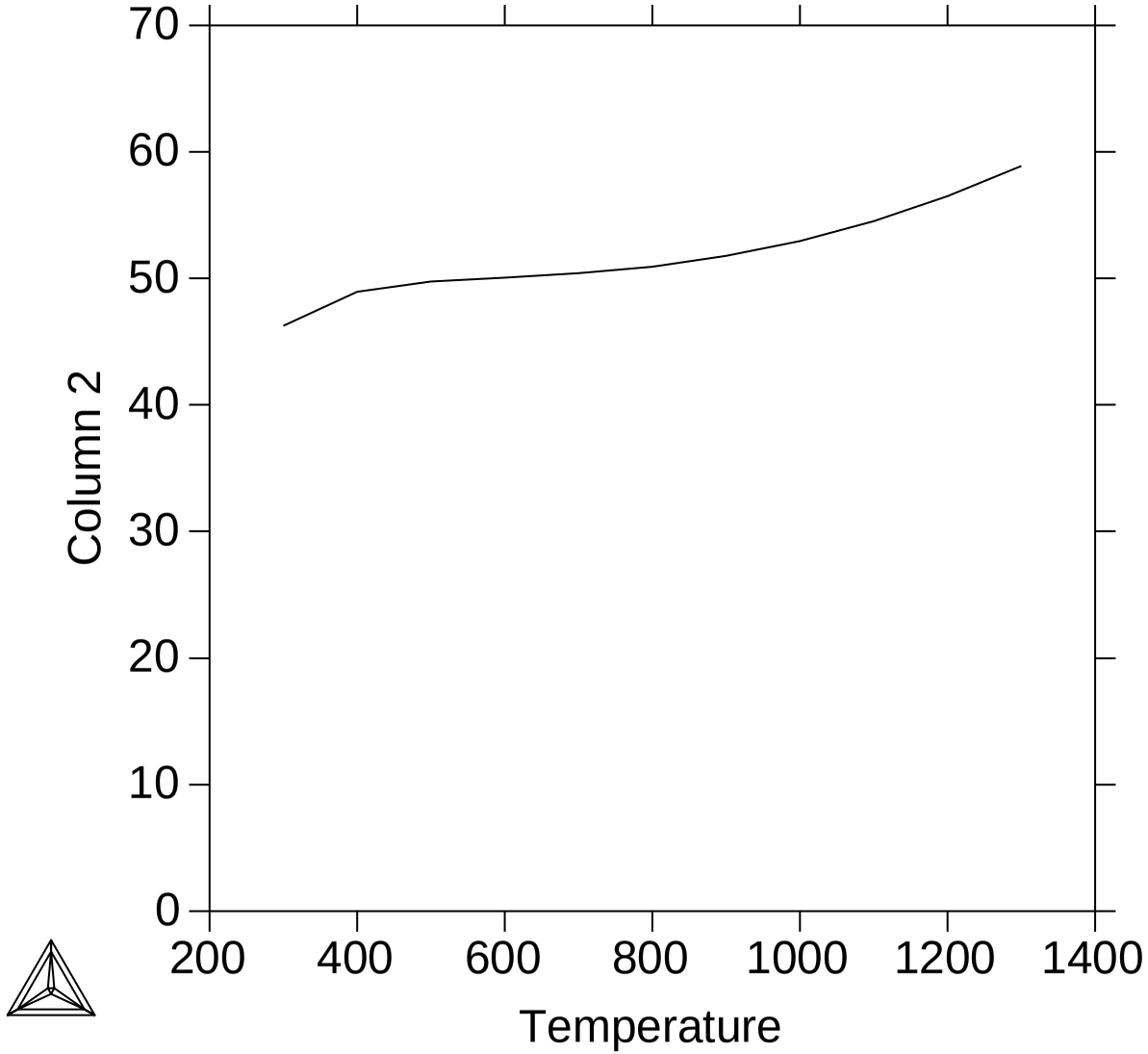
THERMO-CALC (2009.04.15:03.02) :example 12a



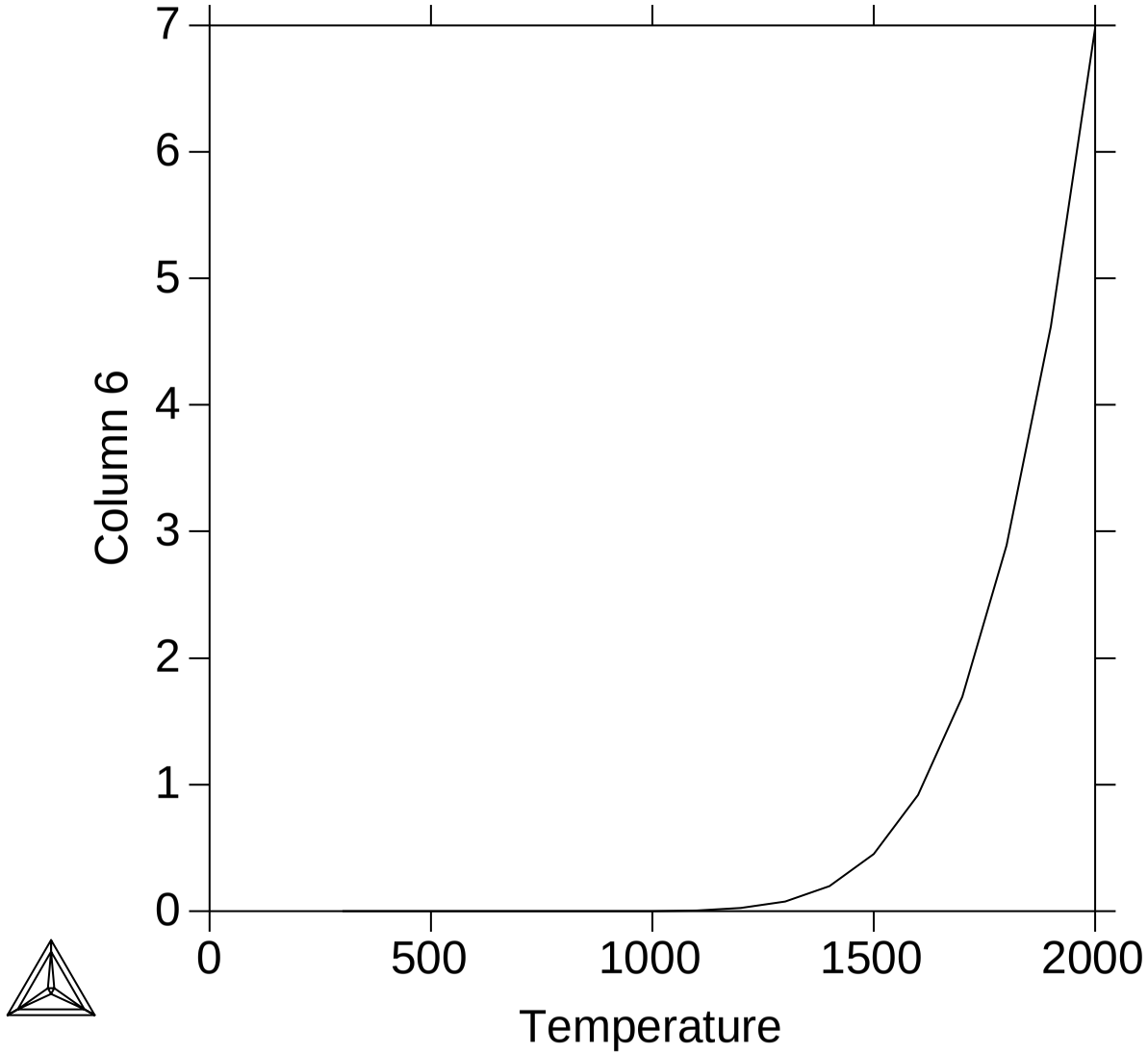
THERMO-CALC (2009.04.15:03.02) :example 12b



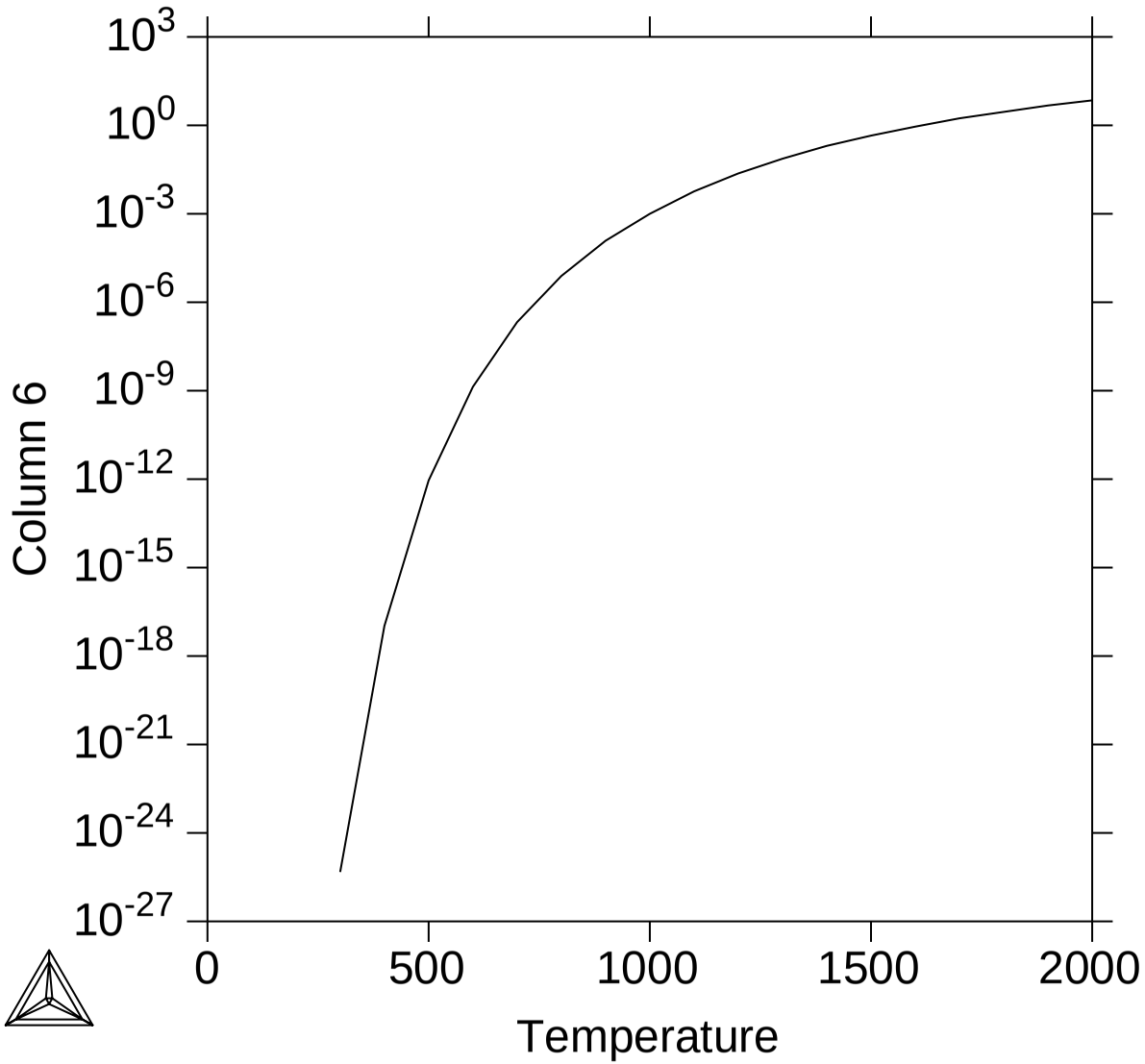
THERMO-CALC (2009.04.15:03.02) :example 12c



THERMO-CALC (2009.04.15:03.02) :example 12d



THERMO-CALC (2009.04.15:03.02) :example 12e



13

Calculation of phase diagram and G curve using the BINARY module

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Binary Al-Cu phase diagram and G curve
SYS: @@
SYS: set-log ex13,,,
SYS: GO BIN
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/:  PBIN
 Current database: TCS Public Binary Alloys TDB v1

 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
First element: ?
 The following assessed systems
    AG-CU   AL-TI   C-CR   C-FE   C-MN   CO-FE   CO-MN   CR-N CO-NI   CR-FE
  FE-O   FE-S   FE-V   C-CO   C-MO   C-NB   C-NI   C-SI   C-V   C-W   CO-CR
  CR-MO   CR-W   FE-MN   FE-MO   FE-N   FE-NB   FE-W   MO-W   N-TI   N-V
  AL-CU   AL-NI   AL-ZN   CU-FE   CU-ZN   PB-SN

First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:
   ... the command in full is REJECT
 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 AL                      TI  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   90Din 'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report
       DMA(A)195, Rev. August 1990'
   91Din 'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, Vol.15,
       No.4, pp.317-425, (1991)'
   NIG-ALTI 'Nigel Saunders, COST 507 round 1, (1991); Al-Ti'
   NIG-ALCU 'Nigel Saunders, COST 507 round 1, (1993); Al-Cu'
   DUP-ALNI 'Nathalie Dupin, J Alloy and Compounds, (1997); Al-Ni'
 -OK-
   ... the command in full is SET_AXIS_VARIABLE
 The condition X(TI)=.1234  created
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=1319.08  created
   ... the command in full is SET_REFERENCE_STATE
   ... the command in full is SET_REFERENCE_STATE
   ... the command in full is SAVE_WORKSPACES
   ... the command in full is SET_CONDITION
```

```
  ... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
  ... the command in full is COMPUTE_EQUILIBRIUM
  ... the command in full is COMPUTE_EQUILIBRIUM
Start points provided by database
  ... the command in full is SAVE_WORKSPACES
Version S mapping is selected

Organizing start points

Generating start point   1
Generating start point   2

Phase region boundary   1 at:   5.740E-01  1.000E+03
 ** TI3AL
    TIAL
*** Buffer saved on file: BINARY.POLY3
Calculated..           30  equilibria
Terminating at axis limit.

Phase region boundary   2 at:   6.006E-01  3.000E+02
 ** TI3AL
    TIAL
Calculated.           45  equilibria

Phase region boundary   3 at:   5.622E-01  1.384E+03
 ** HCP_A3
 ** TI3AL
    TIAL

Phase region boundary   4 at:   5.566E-01  1.384E+03
 ** HCP_A3
    TIAL
Calculated.           15  equilibria

      :
      :
      :

Phase region boundary  26 at:   5.477E-01  1.776E+03
 ** BCC_A2
    HCP_A3
Calculated           46  equilibria

Phase region boundary  27 at:   5.233E-01  1.776E+03
    LIQUID
 ** BCC_A2
Calculated           46  equilibria

Phase region boundary  28 at:   6.013E-01  1.384E+03
 ** HCP_A3
    TI3AL
Calculated..           63  equilibria
Terminating at axis limit.

Phase region boundary  29 at:   5.740E-01  1.000E+03
 ** TI3AL
    TIAL
Calculated.           17  equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: BINARY.POLY3
CPU time for mapping           3  seconds

 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

  ... the command in full is SET_TIELINE_STATUS
  ... the command in full is SET_LABEL_CURVE_OPTION
```

```
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST: @@ Set some phase labels
POST: ADD
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .7 1400
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated         4191  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time    0  s
 Stable phases are: BCC_A2
Text size: /.3400000036/:
POST: ADD
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .51 400
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated         4191  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time    0  s
 Stable phases are: TI3AL+TIAL
Text size: /.3400000036/:
POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,,,,,
POST:
POST: set-title example 13a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ We may plot the activites as well
POST: S-D-A
   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : X
VARIABLE : AC
FOR COMPONENT : AL
POST: s-l e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13b
POST: PLOT
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: S-A-TY X
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: LOG
POST: S-S X N 1E-4 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 13c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Now use inverse of T as y axis
POST: ent fun it=1000/T;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y it
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n .5 1.5
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 13d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Now the G curves for the same system
```

```
POST: BA
   ... the command in full is BACK
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
SYS: GO BIN
   ... the command in full is GOTO_MODULE
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: PBIN
 Current database: TCS Public Binary Alloys TDB v1

 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:  G
Temperature (C): /1000/:  1000
   ... the command in full is REJECT
 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 AL                      TI  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   90Din 'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report
       DMA(A)195, Rev. August 1990'
   91Din 'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, Vol.15,
       No.4, pp.317-425, (1991)'
   NIG-ALTI 'Nigel Saunders, COST 507 round 1, (1991); Al-Ti'
   NIG-ALCU 'Nigel Saunders, COST 507 round 1, (1993); Al-Cu'
   DUP-ALNI 'Nathalie Dupin, J Alloy and Compounds, (1997); Al-Ni'
 -OK-
   ... the command in full is SET_AXIS_VARIABLE
 The condition X(TI)=.1234  created
   ... the command in full is SET_CONDITION
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is SET_REFERENCE_STATE
   ... the command in full is SET_REFERENCE_STATE
   ... the command in full is SAVE_WORKSPACES
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is COMPUTE_EQUILIBRIUM
   ... the command in full is SAVE_WORKSPACES
   ... the command in full is STEP_WITH_OPTIONS

 Phase Region from   0.502463     for:
     LIQUID
     BCC_A2
     FCC_A1
```

```
     HCP_A3
     TI3AL
     TIAL

 Phase Region from   0.502463     for:
     LIQUID
     BCC_A2
     FCC_A1
     HCP_A3
     TI3AL
     TIAL

 Phase Region from   0.320000     for:
     AL11TI5

 Phase Region from   0.333000     for:
     AL2TI

 Phase Region from   0.250000     for:
     AL3M_DO22

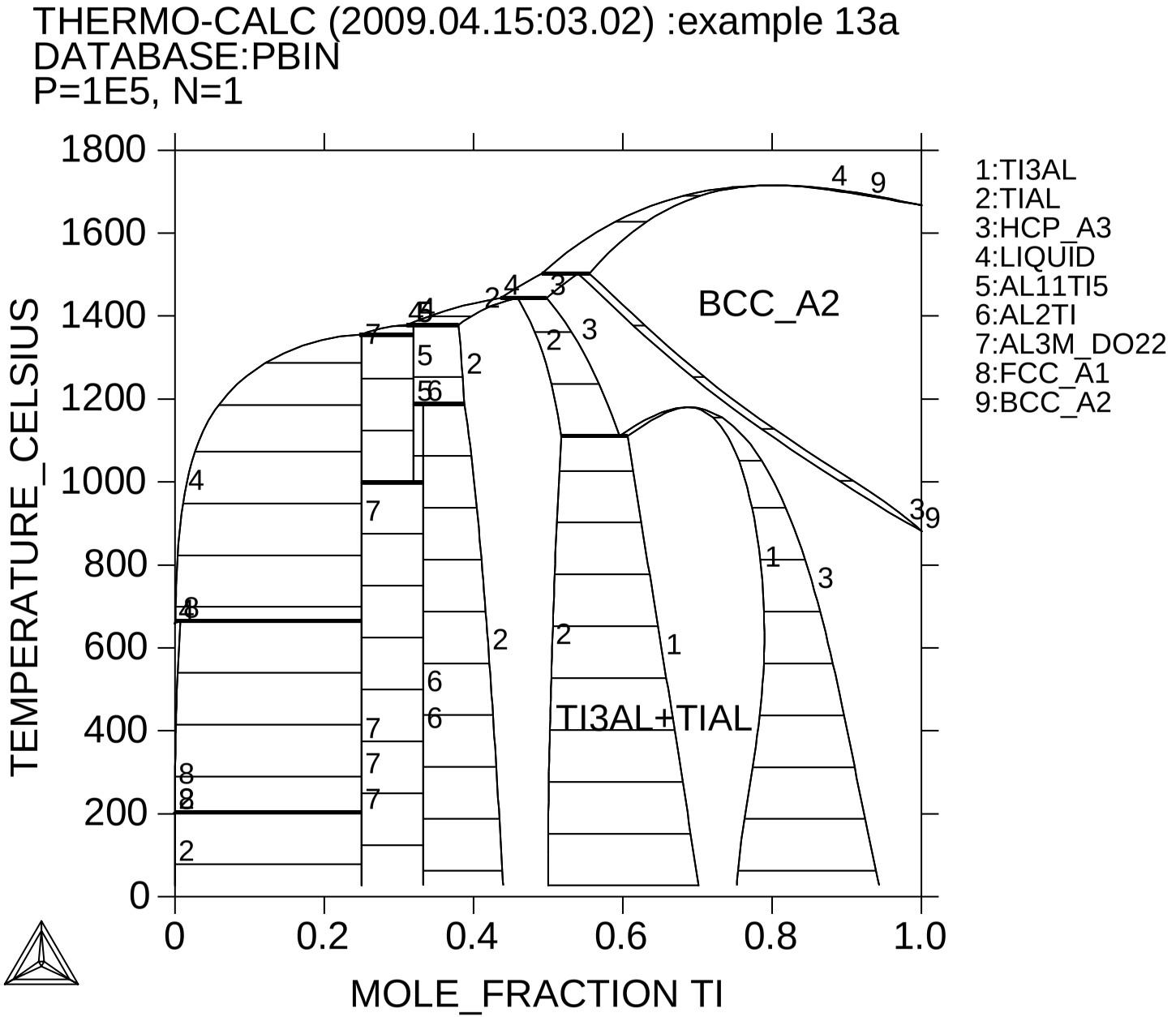
 Phase Region from    0.00000     for:
     AL3NI2

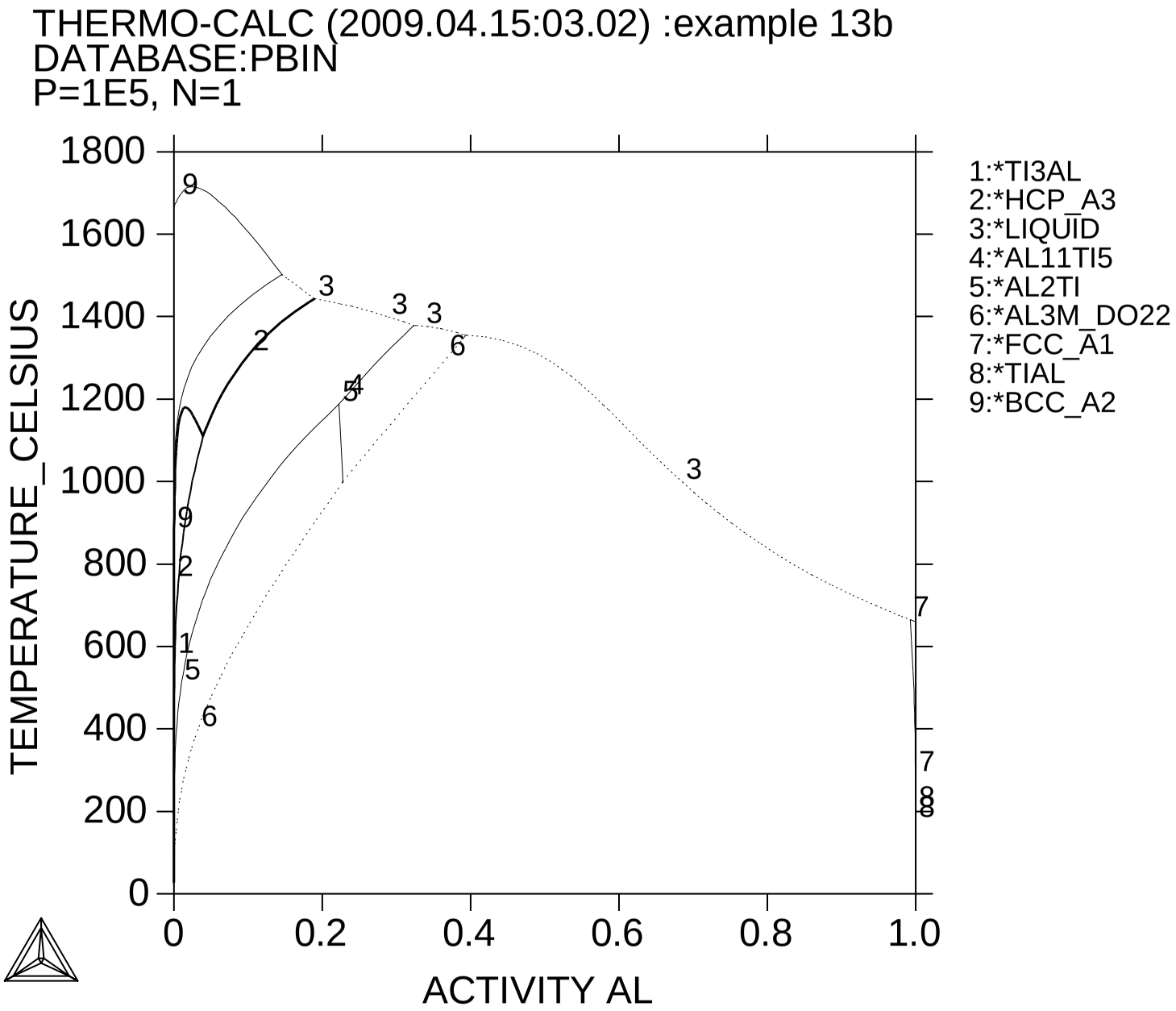
 Phase Region from    0.00000     for:
     ALCU_THETA
 *** Buffer saved on file *** GCURVE.POLY3

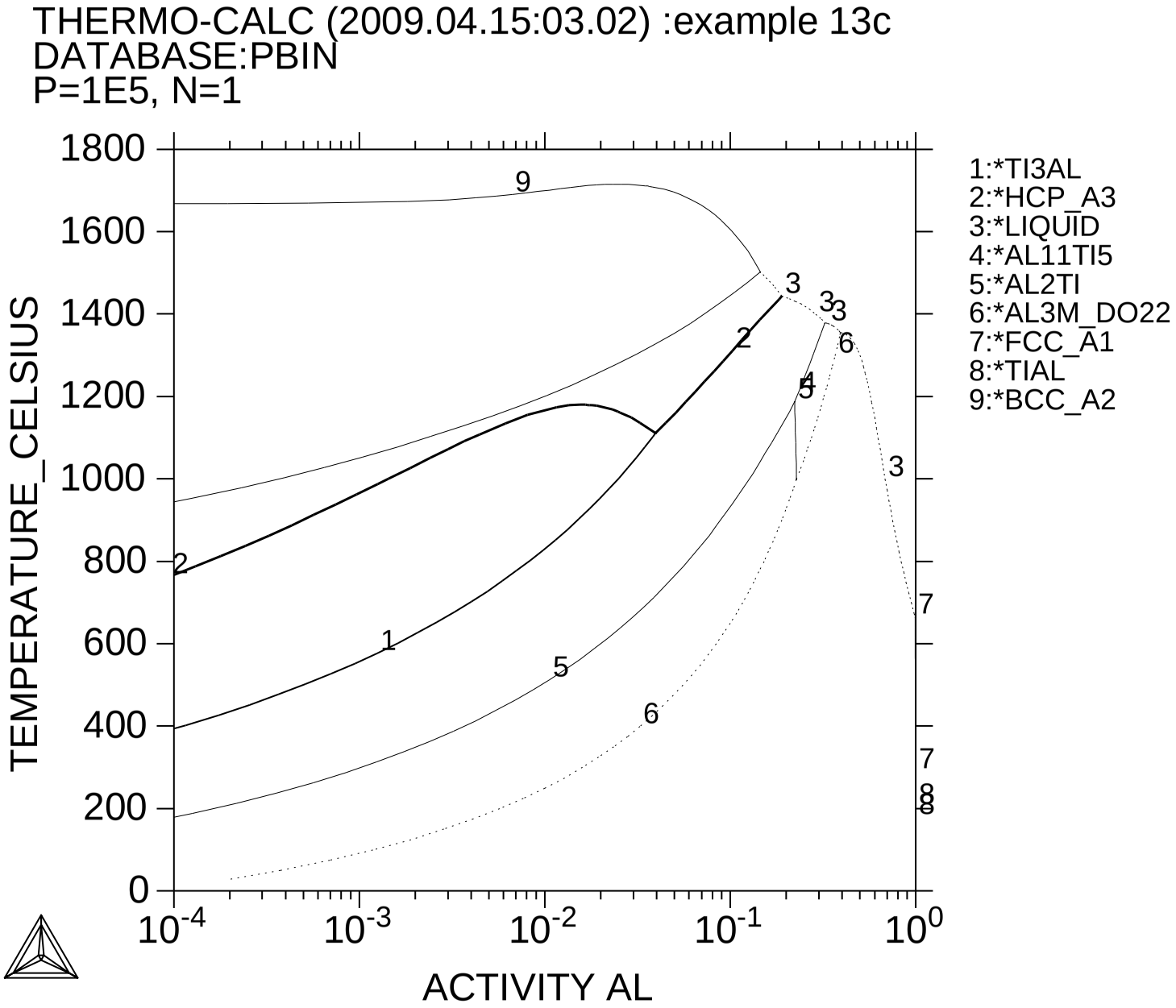
  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

   ... the command in full is SET_TIELINE_STATUS
   ... the command in full is SET_LABEL_CURVE_OPTION
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: s-p-f ##1,,,,,,,,,,
POST:
POST: set-label F
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13e
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
 Current database: TCS Steels/Fe-Alloys Database v6

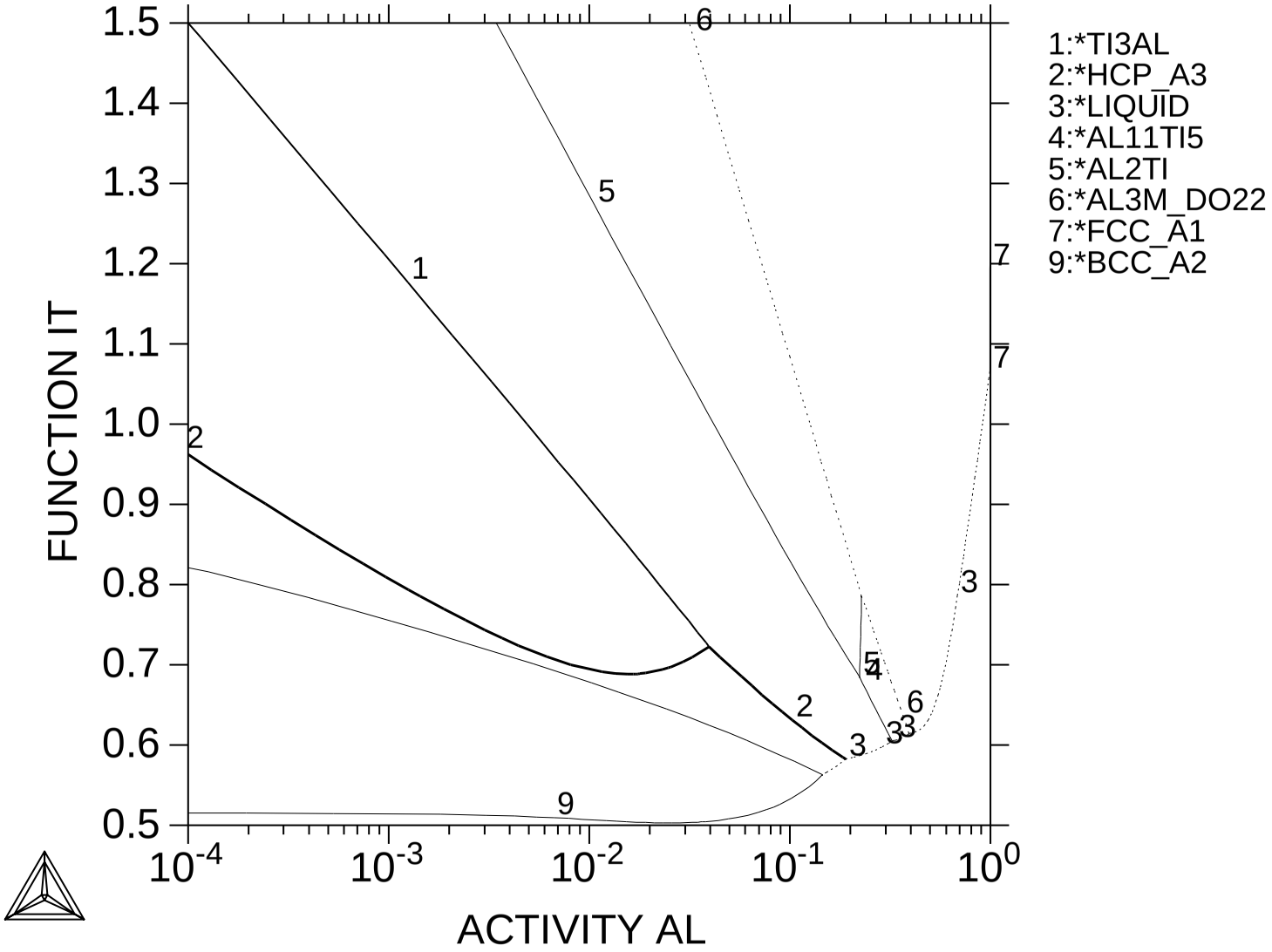
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
SYS: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
SYS: CPU time            5  seconds
```


THERMO-CALC (2009.04.15:03.02) :example 13a
DATABASE:PBIN
P=1E5, N=1
TEMPERATURE_CELSIUS
MOLE_FRACTION TI
BCC_A2
TI3AL+TIAL
1:TI3AL
2:TIAL
3:HCP_A3
4:LIQUID
5:AL11TI5
6:AL2TI
7:AL3M_DO22
8:FCC_A1
9:BCC_A2

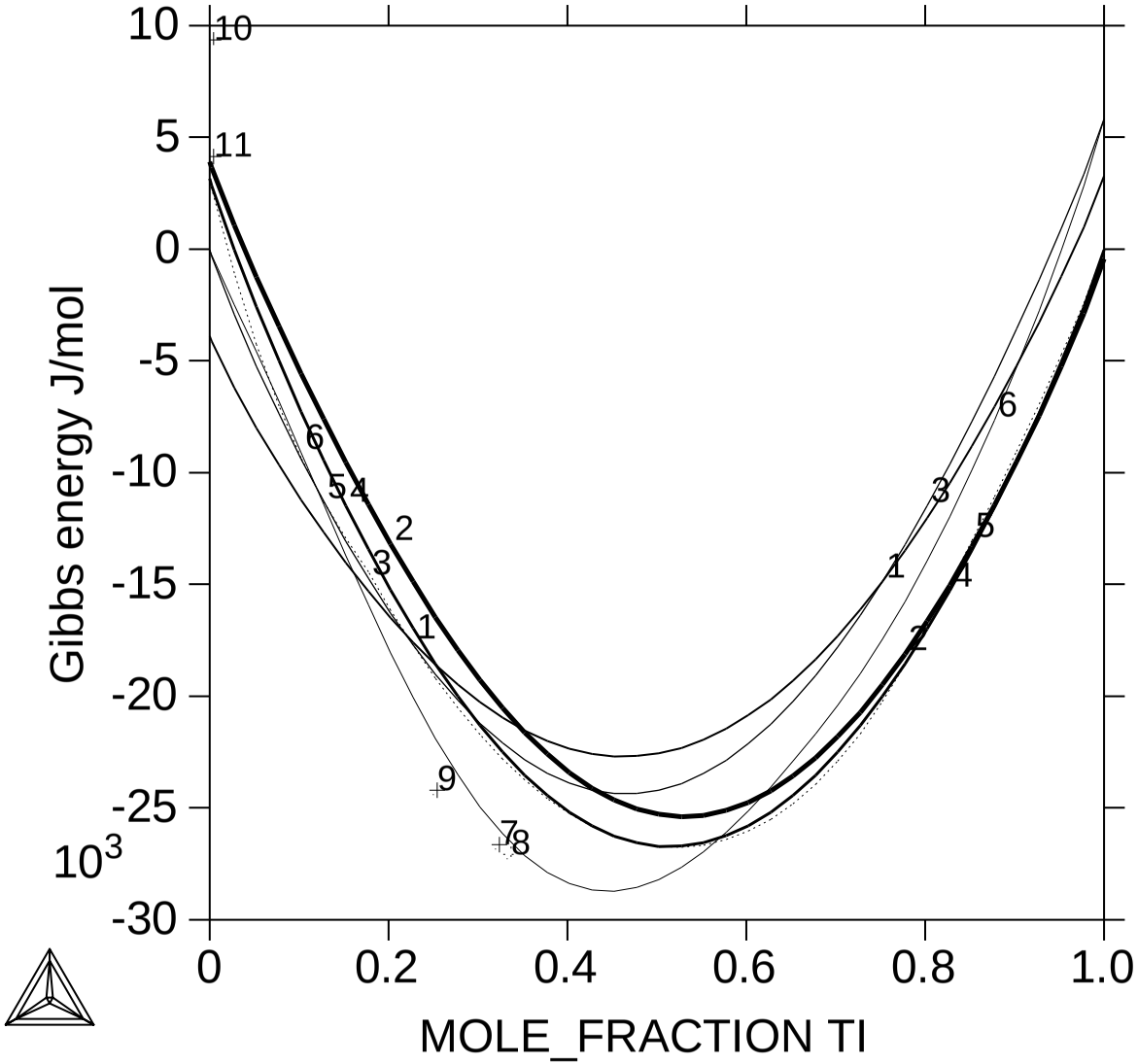

THERMO-CALC (2009.04.15:03.02) :example 13b
DATABASE:PBIN
P=1E5, N=1
TEMPERATURE_CELSIUS
ACTIVITY AL
1800
1600
1400
1200
1000
800
600
400
200
0
0
0.2
0.4
0.6
0.8
1.0
1:*TI3AL
2:*HCP_A3
3:*LIQUID
4:*AL11TI5
5:*AL2TI
6:*AL3M_DO22
7:*FCC_A1
8:*TIAL
9:*BCC_A2


THERMO-CALC (2009.04.15:03.02) :example 13c
DATABASE:PBIN
P=1E5, N=1
TEMPERATURE_CELSIUS
ACTIVITY AL
1800
1600
1400
1200
1000
800
600
400
200
0
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
1:*TI3AL
2:*HCP_A3
3:*LIQUID
4:*AL11TI5
5:*AL2TI
6:*AL3M_DO22
7:*FCC_A1
8:*TIAL
9:*BCC_A2

THERMO-CALC (2009.04.15:03.02) :example 13d
DATABASE:PBIN
P=1E5, N=1



THERMO-CALC (2009.04.15:03.02) :example 13e
DATABASE:PBIN
P=1E5, N=1, T=1273.15;



1:X(TI),GMR(LIQUID)
2:X(TI),GMR(BCC_A2)
3:X(TI),GMR(FCC_A1)
4:X(TI),GMR(HCP_A3)
5:X(TI),GMR(TI3AL)
6:X(TI),GMR(TIAL)
7:X(TI),GMR(AL11TI5)
8:X(TI),GMR(AL2TI)
9:X(TI),GMR(AL3M_DO22)
10:X(TI),GMR(AL3NI2)
11:X(TI),GMR(ALCU_THETA)

14

Calculation of heat and heat capacity variations during solidification of an Al-Mg-Si alloy

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of the variation of the heat and the heat capacity
SYS: @@ during solidification of an Al-Mg-Si alloy
SYS: @@
SYS: set-log ex14,,,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw PTERN
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN: d-sys al mg si
   ... the command in full is DEFINE_SYSTEM
 AL                      MG                      SI
   DEFINED
TDB_PTERN: l-s c
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :AL MG SI:
  > This is metallic liquid solution phase, with C species
 FCC_A1      :AL MG SI:VA:
 HCP_A3      :AL MG SI:VA:
 DIAMOND_A4  :AL SI:
 ALMG_BETA   :AL:MG:
 ALMG_DZETA  :AL:MG:
 ALMG_EPSILON :AL:MG:
 AL12MG17    :MG:AL MG:AL MG:
 MG2SI       :MG:SI:
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'N Saunders, COST project (1994); MG-SI'
  'H L Lukas, COST project (1994); AL-SI'
  'H L Lukas, COST project (1994); MG-SI'
  'H L Lukas, COST project (1994); AL-MG-SI'
 -OK-
TDB_PTERN: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ The composition
POLY_3: s-c w(si)=.09,w(mg)=.15,t=1000,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(SI)=9E-2, W(MG)=0.15, T=1000, P=1E5, N=1
 DEGREES OF FREEDOM 0
```

```
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7891  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: PTERN

 Conditions:
 W(SI)=9E-2, W(MG)=0.15, T=1000, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.66361E+01
 Total Gibbs energy -4.84600E+04,  Enthalpy  3.06712E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      7.5026E-01  7.6000E-01 4.6614E-03 -4.4636E+04 SER
 MG                      1.6439E-01  1.5000E-01 3.1193E-04 -6.7121E+04 SER
 SI                      8.5357E-02  9.0000E-02 3.8932E-03 -4.6133E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.6636E+01, Volume fraction 0.0000E+00  Mass fractions:
 AL  7.60000E-01  MG  1.50000E-01  SI  9.00000E-02
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Set termperature as axis
POLY_3: s-a-v
   ... the command in full is SET_AXIS_VARIABLE
Axis number: /1/:  1
Condition /NONE/:  t
Min value /0/:  500
Max value /1/:  1000
Increment /12.5/:  12.5
POLY_3: save tcex14 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    1000.00
 Global calculation of initial equilibrium ....OK

 Phase Region from    1000.00     for:
     LIQUID
 Global check of adding phase at  9.50336E+02
 Calculated     7 equilibria

 Phase Region from    950.336     for:
     LIQUID
     MG2SI
 Global test at  8.80000E+02 .... OK
 Global check of adding phase at  8.66207E+02
 Calculated    12 equilibria

 Phase Region from    866.207     for:
     LIQUID
     FCC_A1
     MG2SI
 Global check of removing phase at  8.47625E+02
 Calculated     5 equilibria

 Phase Region from    847.625     for:
     FCC_A1
     MG2SI
 Global test at  7.70000E+02 .... OK
 Global check of adding phase at  7.39271E+02
 Calculated    14 equilibria

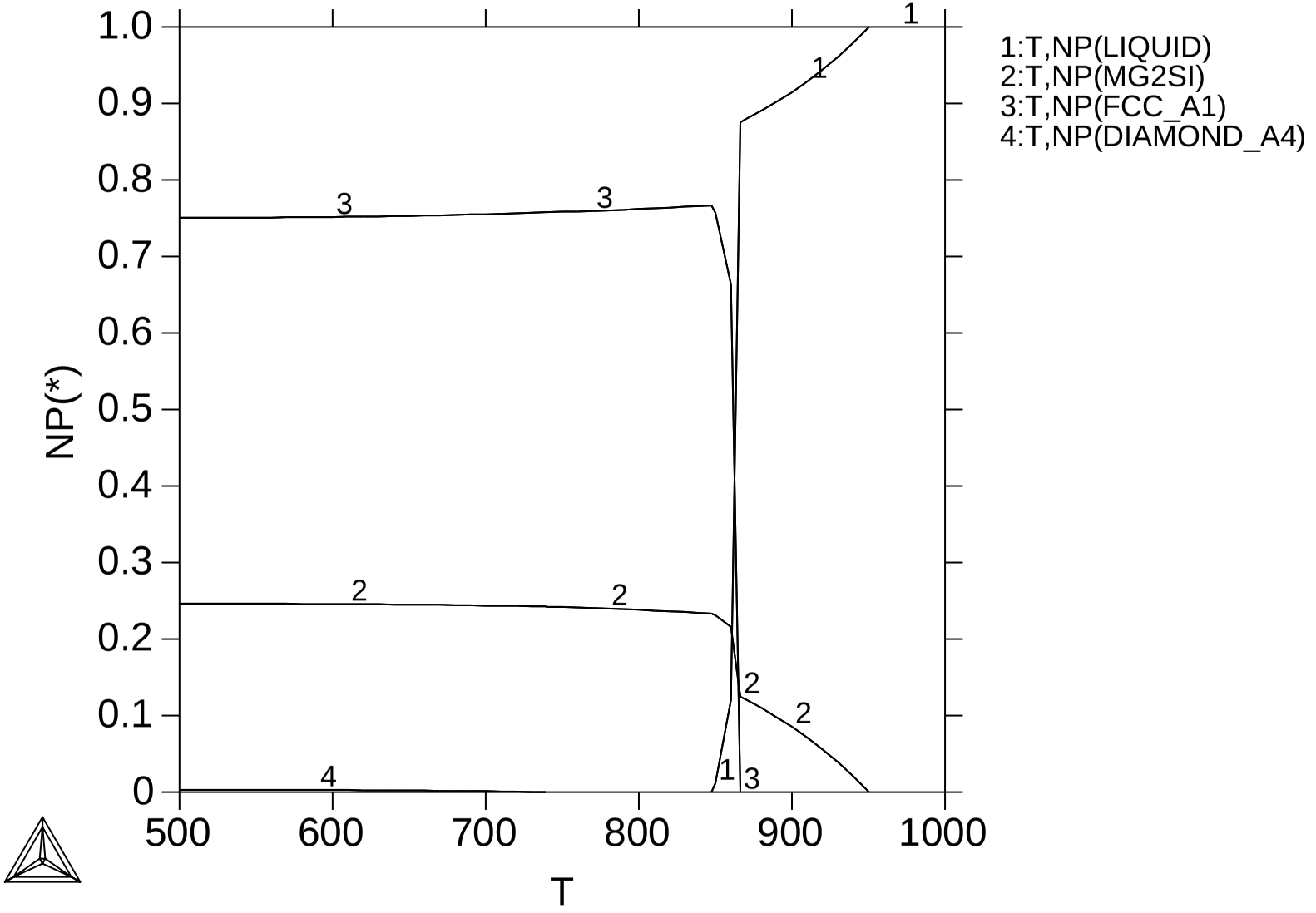
 Phase Region from    739.271     for:
     DIAMOND_A4
```

```
     FCC_A1
     MG2SI
 Global test at  6.60000E+02 .... OK
 Global test at  5.60000E+02 .... OK
 Terminating at    500.000
 Calculated    27 equilibria
 *** Buffer saved on file: tcex14.POLY3
POLY_3: POST
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

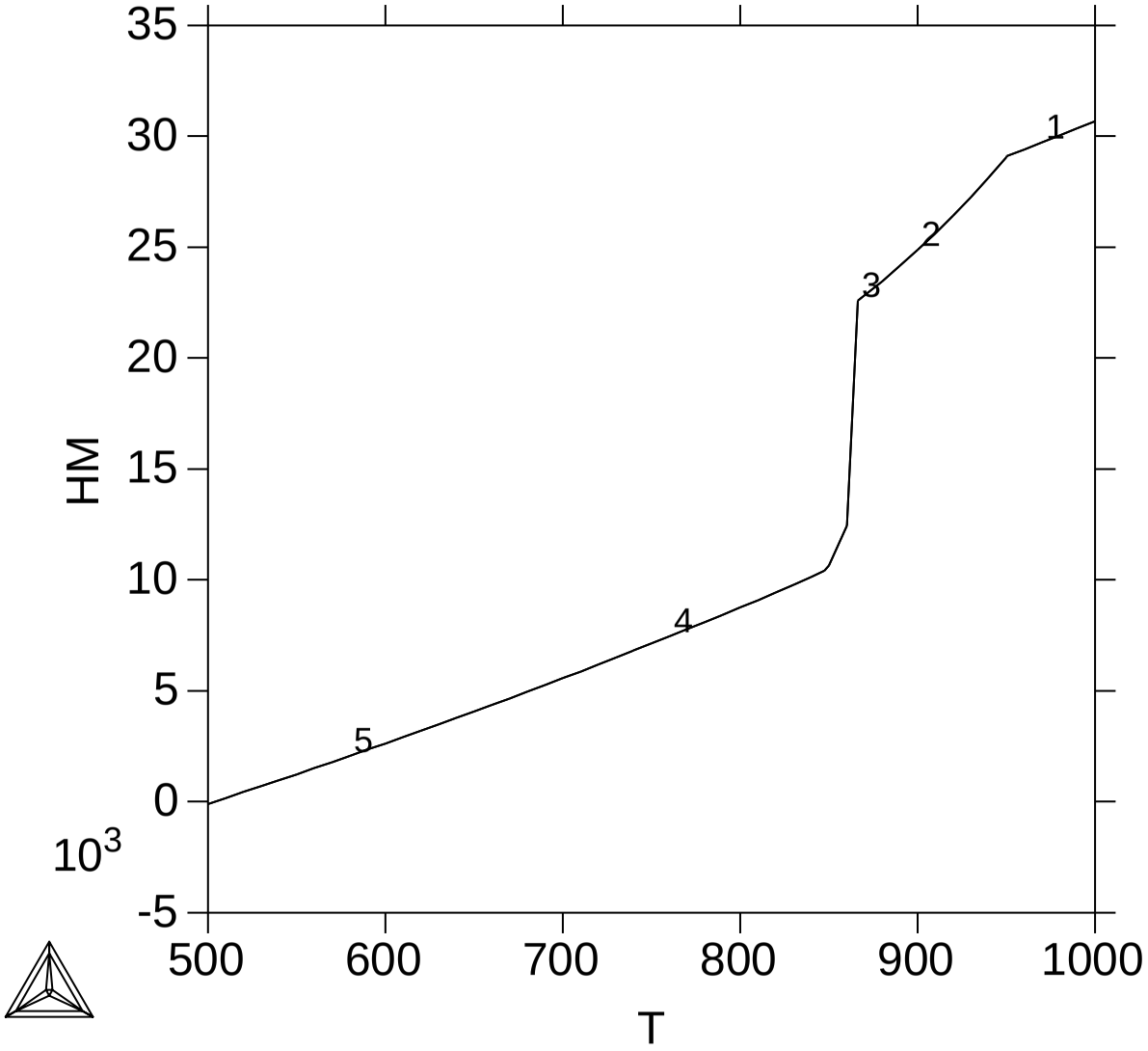
 Setting automatic diagram axis

POST: @@ Plot phase fractions
POST: S-D-A X T
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y NP(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: S-LAB D
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 14a
POST: PLOT
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Plot the total enthalpy (heat)
POST: S-D-A Y HM
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-LAB B
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 14b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Plot the heat capacity. This must first be entered as
POST: @@ a function as derivatives cannot be plotted directly.
POST: ENT FUN CP=HM.T;
   ... the command in full is ENTER_SYMBOL
POST: S-D-A Y CP
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-S
   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC SCALING  (Y OR N) /N/:  N
MIN VALUE : 0
MAX VALUE : 140
POST: S-A-T-S
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC AXIS TEXT  (Y OR N) /N/:  N
AXIS TEXT : HEAT CAPACITY (J/MOL/K)
POST: set-title example 14c
POST: PLOT
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           2  seconds
```

THERMO-CALC (2009.04.15:03.02) :example 14a
DATABASE:PTERN
W(SI)=9E-2, W(MG)=0.15, P=1E5, N=1.;

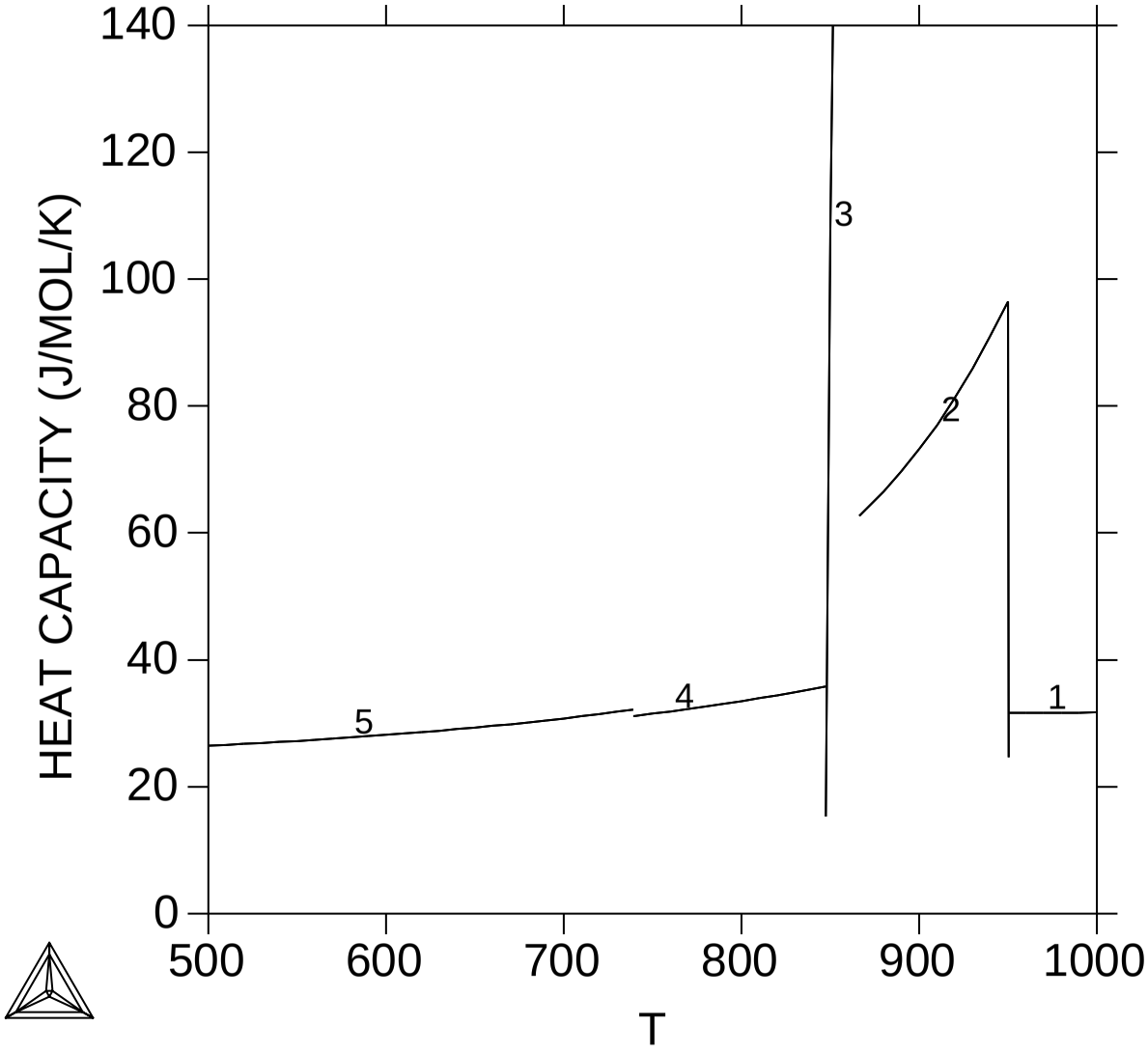


THERMO-CALC (2009.04.15:03.02) :example 14b
DATABASE:PTERN
W(SI)=9E-2, W(MG)=0.15, P=1E5, N=1.;



1: LIQUID
2: LIQUID MG2SI
3: LIQUID FCC_A1 MG2SI
4: FCC_A1 MG2SI
5: DIAMOND_A4 FCC_A1 MG2SI

THERMO-CALC (2009.04.15:03.02) :example 14c
DATABASE:PTERN
W(SI)=9E-2, W(MG)=0.15, P=1E5, N=1.;



1: LIQUID
2: LIQUID MG2SI
3: LIQUID FCC_A1 MG2SI
4: FCC_A1 MG2SI
5: DIAMOND_A4 FCC_A1 MG2SI

15

Solidification simulation of a Cr-Ni alloy using the SCHEIL module

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ This is an example of a solidification simulation of a Cr-Ni alloy.
SYS: @@ No back diffusion in the solid, i.e. Scheil-Gulliver model.
SYS: @@
SYS: SET-LOG ex15,,,
SYS: GO SCHEIL
   ... the command in full is GOTO_MODULE

         SCHEIL_GULLIVER SIMULATION MODULE VERSION 4.0

 ..........................................................
 .                                                        .
 .        1. Start new simulation                         .
 .        2. Open old file and plot diagram               .
 .        3. Open old file and make another simulation     .
 .                                                        .
 ..........................................................

Select option /1/: 1
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/: TCFE6
Major element or alloy: cr
Composition input in mass (weight) percent? /Y/: n
 Composition will be taken to be in mole percent
1st alloying element: ni 10
2nd alloying element:
Temperature (C) /2000/: 2000
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED

 This database has following phases for the defined system

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  SIGMA                   CHI_A12
 LAVES_PHASE_C14         CR3SI                   NBNI3
 NI3TI

Reject phase(s) /NONE/: *
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  SIGMA                   CHI_A12
 LAVES_PHASE_C14         CR3SI                   NBNI3
 NI3TI  REJECTED
Restore phase(s):: liq fcc bcc
 LIQUID:L                FCC_A1                  BCC_A2
   RESTORED
Restore phase(s): /NONE/:

 ..................................................

    The following phases are retained in this system:

 LIQUID:L                BCC_A2                  FCC_A1
```

```
 ..................................................

OK? /Y/:  y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, pp. 1155-1170'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
 -OK-
Should any phase have a miscibility gap check? /N/:  n
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
     Calculated liquidus temperature is 1786.00(C)
     Please enter simulation conditions !

Temperature step (C) /1/:  5
Default stop point? /Y/:  y
Fast diffusing components: /NONE/:  none
Buffer-saving file name /scheil/:
   ... the command in full is ADD_INITIAL_EQUILIBRIUM

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

   ... the command in full is ADVANCED_OPTIONS
   ... the command in full is STEP_WITH_OPTIONS

 Phase Region from    2059.15     for:
     LIQUID
 Calculated     4 equilibria

 Phase Region from    2058.59     for:
     LIQUID
     BCC_A2
 Calculated    35 equilibria

 Phase Region from    1897.34     for:
     BCC_A2
 *** Buffer saved on file: scheil.POLY3

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is ENTER_SYMBOL
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 An EXP file scheil_EQ.EXP
 has been created to store the equilibrium            solidification results.
   ... the command in full is READ_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

   ... the command in full is ADD_INITIAL_EQUILIBRIUM
```

```
 Phase Region from    2059.15     for:
     LIQUID
 Calculated     4 equilibria

 Phase Region from    2058.59     for:
     LIQUID
     BCC_A2

 Phase Region from    1617.95     for:
     LIQUID
     BCC_A2
     FCC_A1
 Calculated    91 equilibria

 Phase Region from    1617.95     for:
     BCC_A2
     FCC_A1
 Calculated     3 equilibria
 *** Buffer saved on file: scheil.POLY3
   ... the command in full is REINITIATE_PLOT_SETTINGS

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is SET_AUTOMATIC_DIAGRAM_A

 Setting automatic diagram axis

   ... the command in full is APPEND_EXPERIMENTAL_DATA
Hard copy of the diagram? /N/:  n
Save coordinates of curve on text file? /N/:  n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
   ... the command in full is SET_LABEL_CURVE_OPTION
Any more diagrams? /Y/:

  ..........................................................

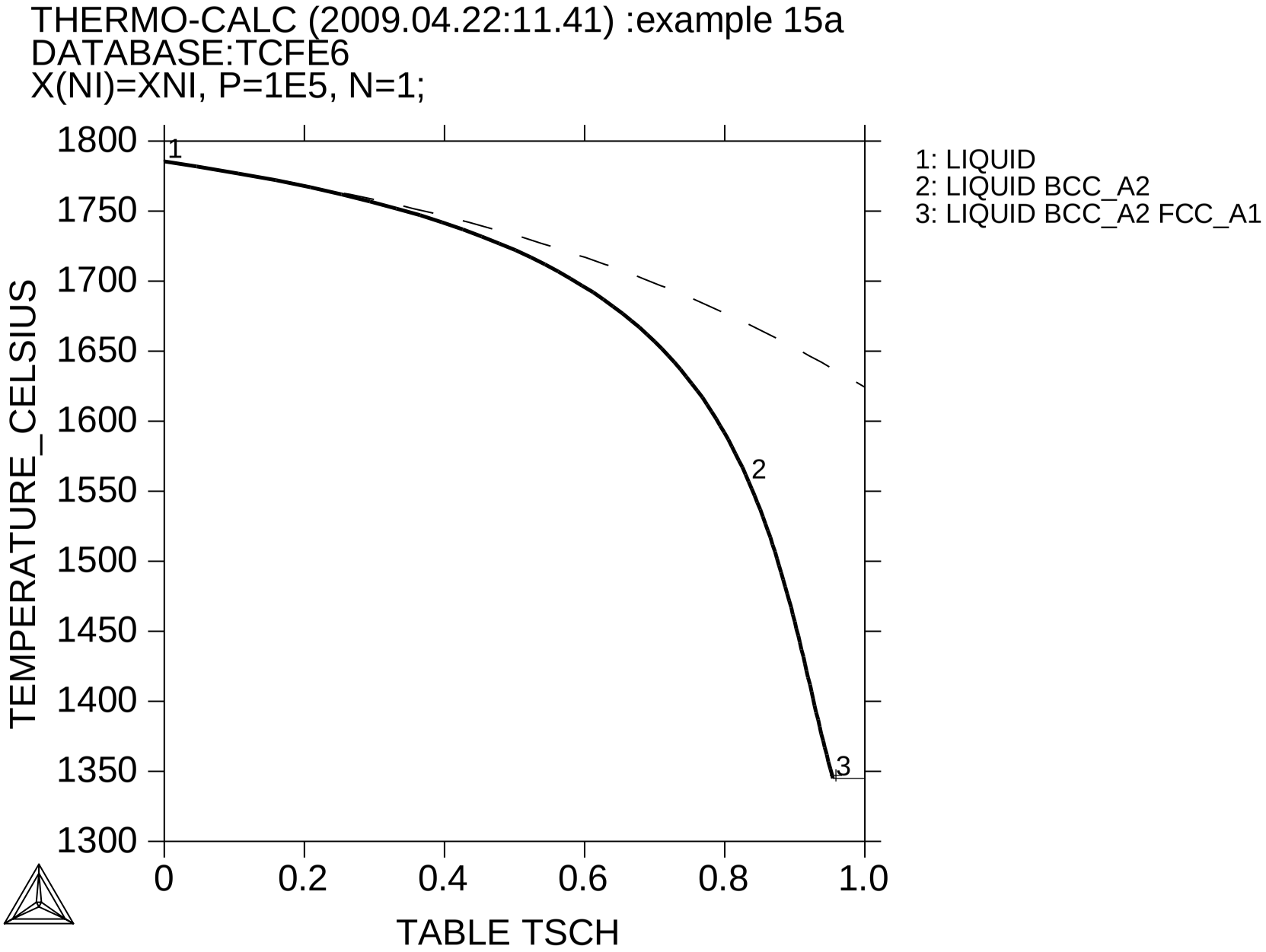
        The following axis variables are available

             T --- Temperature in Celsius
         NL/BL --- Mole/mass fraction of liquid
         NS/BS --- Mole/mass fraction of all solid phases
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
      W(ph,el) --- Weight fraction of an element in a phase
      X(ph,el) --- Mole fraction of an element in a phase
      Y(ph,el) --- Site fraction of an element in a phase
     NN(ph,el) --- Distribution of an element in a phases
         NH/BH --- Heat release and Latent heat per mole/gram
        CP/BCP --- Apparent heat capacity per mole/gram
     NV/NV(ph) --- Molar volume of the system or a phase
     DS/DS(ph) --- Average density of the system or a phase
            BT --- Apparent volumetric TEC of the system

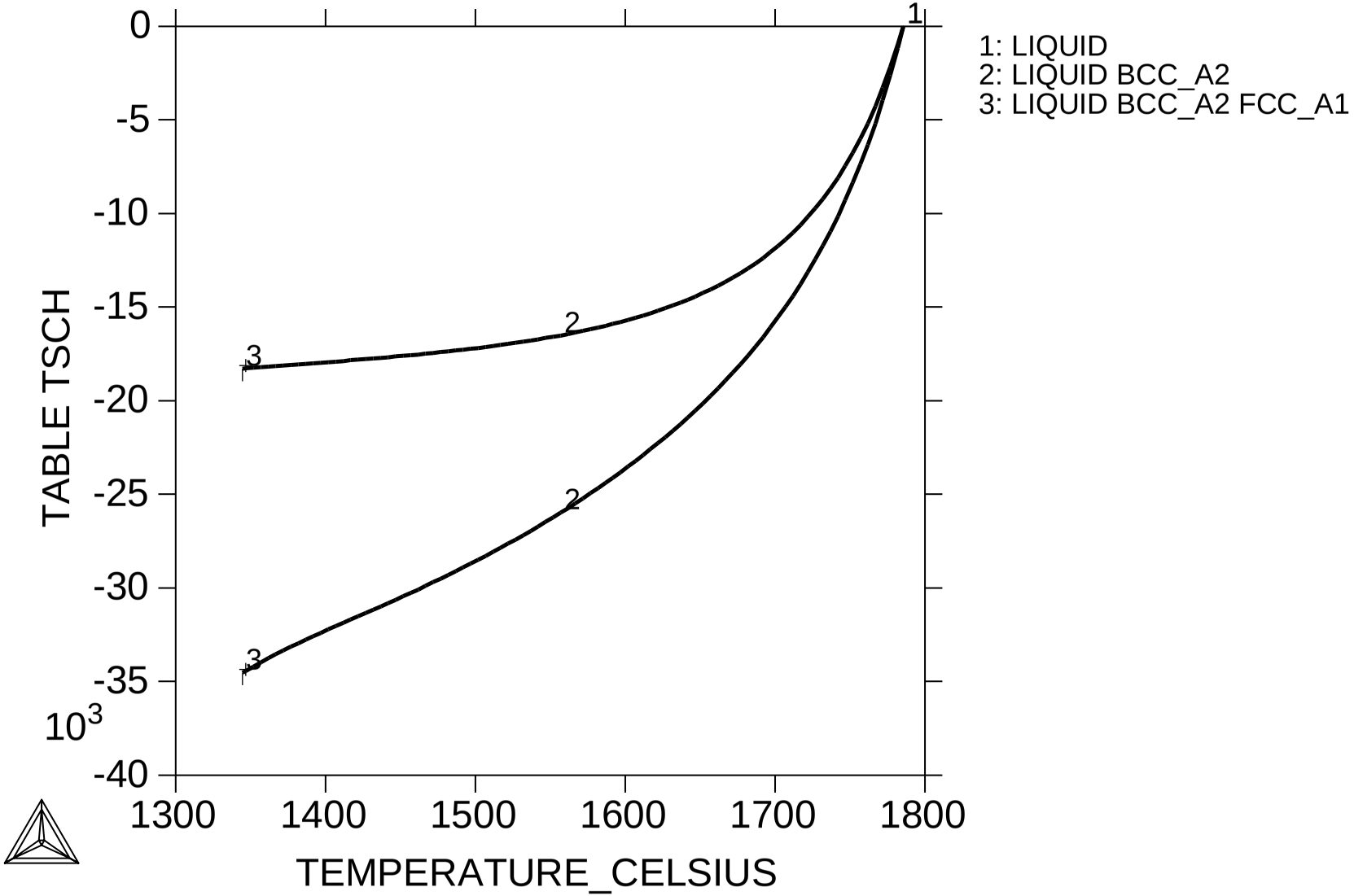
  "el" and "ph" are name of element and phase, respectively
     "*" can be used as a wild character for "el" and "ph"

  ..........................................................

X-axis Variable: t
Y-axis Variable: nh
Zoom in? /N/:  n
Hard copy of the diagram? /N/:  n
Save coordinates of curve on text file? /N/:  n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
   ... the command in full is SET_LABEL_CURVE_OPTION
Any more diagrams? /Y/:  n
   ... the command in full is ADVANCED_OPTIONS
SYS: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
SYS:SYS: CPU time            2  seconds
```


THERMO-CALC (2009.04.22:11.41) :example 15a
DATABASE:TCFE6
X(NI)=XNI, P=1E5, N=1;
1800
1750
1700
1650
1600
1550
1500
1450
1400
1350
1300
TEMPERATURE_CELSIUS
0
0.2
0.4
0.6
0.8
1.0
TABLE TSCH
1
2
3
1: LIQUID
2: LIQUID BCC_A2
3: LIQUID BCC_A2 FCC_A1

THERMO-CALC (2009.04.22:11.51) :example 15b
DATABASE:TCFE6
X(NI)=XNI, P=1E5, N=1;



16

Calculation of the second order transition line in the Bcc field of the Al-Fe system

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of a second order transition line in Al-Fe
SYS: @@
SYS: SET-LOG ex16,,
SYS: GO D
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: SW SSOL2
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Alloy Solutions Database v2

 VA  DEFINED
 B2_BCC                  L12_FCC                 AL5FE4:
   REJECTED
 GAS:G                   AQUEOUS:A               WATER:A
   REJECTED
TDB_SSOL2: D-SYS AL FE
   ... the command in full is DEFINE_SYSTEM
 AL                      FE  DEFINED
TDB_SSOL2: REJ PH /ALL
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  CBCC_A12                CUB_A13
 FE4N                    AL13FE4                 AL2FE
 AL5FE2                  TI3AL                   TIAL
 AL3NI2                  ALNI_B2                 ALCU_THETA
   REJECTED
TDB_SSOL2: @@ The BCC phase has B2 ordering in this system
TDB_SSOL2: @@ Note that this is modelled with two sublattices
TDB_SSOL2: @@ with both components in both sublattices
TDB_SSOL2: REST PH LIQ B2 BCC
   ... the command in full is RESTORE
 LIQUID:L                B2_BCC                  BCC_A2
   RESTORED
TDB_SSOL2: LI-SYS
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 LIQUID:L    :AL FE:
  > Liquid solution, mainly metallic but also with CaO-SiO2
 BCC_A2      :AL FE:VA:
 B2_BCC      :AL FE:AL FE:VA:
  > This is B2, the ordered BCC phase
TDB_SSOL2: GET
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
   'Marion Seiersten, unpublished work (1989); Al-Fe'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
       September 1989'
 UNARY G0 PARAMETERS ARE MISSING
```

```
 BINARY L0 PARAMETERS ARE MISSING
 CHECK THE FILE MISSING.LIS FOR COMPLETE INFO
 -OK-
TDB_SSOL2: GO P-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3:
POLY_3: adv g n n
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY_3:
POLY_3: @@ Set conditions where the B2 phase should be ordered
POLY_3: SET-COND P=1E5,N=1,T=400,X(AL)=.4
   ... the command in full is SET_CONDITION
POLY_3: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    21 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Use option N in order to see how Al and Fe distribute
POLY_3: @@ on the sublattices
POLY_3: LIST-EQ
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  N
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL2

 Conditions:
 P=1E5, N=1, T=400, X(AL)=0.4
 DEGREES OF FREEDOM 0

 Temperature    400.00 K (   126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.43008E+01
 Total Gibbs energy -3.81516E+04,  Enthalpy -2.55845E+04,  Volume  4.27477E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      4.0000E-01  2.4362E-01 4.1865E-08 -5.6501E+04 SER
 FE                      6.0000E-01  7.5638E-01 4.1257E-04 -2.5918E+04 SER

 B2_BCC                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.4301E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  7.56379E-01  AL  2.43621E-01
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  9.99996E-01  AL  4.22881E-06
 Sublattice  2,  Number of sites  5.0000E-01
 AL  7.99996E-01  FE  2.00004E-01
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Change the condition of Al amount to be that the site-fractions
POLY_3: @@ in the two sublattices will have a certain difference. If they
POLY_3: @@ are the same the B2 phase is disordered
POLY_3: SET-COND X(AL)=NONE
   ... the command in full is SET_CONDITION
POLY_3: SET-COND Y(B2_BCC,FE#1)-Y(B2_BCC,FE#2)=0.1
   ... the command in full is SET_CONDITION
POLY_3: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
    26 ITS,  CPU TIME USED   0 SECONDS
POLY_3: LIST-EQ
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWNS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL2

 Conditions:
 P=1E5, N=1, T=400, Y(B2_BCC,FE)-Y(B2_BCC,FE#2)=0.1
 DEGREES OF FREEDOM 0

 Temperature    400.00 K (   126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.36842E+01
 Total Gibbs energy -1.86969E+04,  Enthalpy -4.69408E+03,  Volume  6.59079E-06
```

```
 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      7.4926E-02  3.7658E-02 7.3603E-14 -1.0057E+05 SER
 FE                      9.2507E-01  9.6234E-01 2.6575E-02 -1.2065E+04 SER

 B2_BCC                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3684E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  9.62342E-01  AL  3.76578E-02
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  9.75074E-01  AL  2.49265E-02
 Sublattice  2,  Number of sites  5.0000E-01
 FE  8.75074E-01  AL  1.24926E-01
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Set the difference smaller. This is as close to the second order
POLY_3: @@ transition as it is possible to be
POLY_3: SET-COND Y(B2_BCC,FE#1)-Y(B2_BCC,FE#2)=1E-4
   ... the command in full is SET_CONDITION
POLY_3: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
    14 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Now vary the temperature using these conditions
POLY_3: SET-AXIS-VAR 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/:  T
Min value /0/:  400
Max value /1/:  2000
Increment /40/:  10
POLY_3: @@ Always save before STEP or MAP (unless you want to overlay the new
POLY_3: @@ results on some previous results)
POLY_3: SAVE tcex16 Y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: STEP NORMAL
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    400.000
 POLY has calculated initial equilibrium

 Phase Region from    400.000     for:
     B2_BCC
 Calculated   127 equilibria

 Phase Region from    1645.23     for:
     LIQUID
     B2_BCC
 Calculated     3 equilibria

 Phase Region from    1645.23     for:
     B2_BCC
 Calculated     3 equilibria

 Phase Region from    1645.23     for:
     LIQUID
     B2_BCC
 Calculated     3 equilibria
 Sorry cannot continue     0 189 1    1.6452267E+03
 *** Buffer saved on file: tcex16.POLY3
POLY_3: POST
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: SET-DIA-AXIS X X(B2_BCC,FE)
   ... the command in full is SET_DIAGRAM_AXIS
POST: SET-DIA-AXIS Y T-K
   ... the command in full is SET_DIAGRAM_AXIS
POST: SET-SCAL X N 0 1
```

```
   ... the command in full is SET_SCALING_STATUS
POST: SET-SCAL Y N 400 2000
   ... the command in full is SET_SCALING_STATUS
POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,
POST:
POST: set-title example 16a
POST: PLOT
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Write on file for plotting together with phase diagram
POST: MAKE TCEX16
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
FILE EXISTS, OVERWRITE (Y OR N) /N/:  Y
POST: BACK
POLY_3: GO D
   ... the command in full is GOTO_MODULE
TDB_SSOL2: @@ Get data for all phases stable in Al-Fe
TDB_SSOL2: REJ-SYS
   ... the command in full is REJECT
 VA  DEFINED
 B2_BCC                 L12_FCC                AL5FE4:
   REJECTED
 GAS:G                  AQUEOUS:A              WATER:A
   REJECTED
 REINITIATING GES5 .....
TDB_SSOL2: D-SYS AL FE
   ... the command in full is DEFINE_SYSTEM
 AL                     FE  DEFINED
TDB_SSOL2: L-SYS
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/:  CONSTITUENT
 LIQUID:L    :AL FE:
  > Liquid solution, mainly metallic but also with CaO-SiO2
 FCC_A1      :AL FE:VA:
  > This is also the MC(1-x) carbide or nitride
 BCC_A2      :AL FE:VA:
 HCP_A3      :AL FE:VA:
  > This is also the M2C carbide and M2N nitride
 CBCC_A12    :AL FE:VA:
  > This is also the alpha-Mn phase
 CUB_A13     :AL FE:VA:
  > This is also the beta-Mn phase
 FE4N        :FE:VA:
 AL13FE4     :AL:FE:AL VA:
 AL2FE       :AL:FE:
 AL5FE2      :AL:FE:
 TI3AL       :AL:AL:
 TIAL        :AL:AL:
 AL3NI2      :AL:AL:
  >This is the ordered HCP phase in Al-Ni
 ALNI_B2     :VA:AL:
  >This is the B2 phase in Al-Ni
 ALCU_THETA  :AL:AL:
TDB_SSOL2: REJ PH /ALL
   ... the command in full is REJECT
 LIQUID:L               FCC_A1                 BCC_A2
 HCP_A3                 CBCC_A12               CUB_A13
 FE4N                   AL13FE4                AL2FE
 AL5FE2                 TI3AL                  TIAL
 AL3NI2                 ALNI_B2                ALCU_THETA
   REJECTED
TDB_SSOL2: REST PH LIQ FCC B2 BCC AL13FE4 AL2FE AL5FE2 AL5FE4
   ... the command in full is RESTORE
 LIQUID:L               FCC_A1                 B2_BCC
 BCC_A2                 AL13FE4                AL2FE
 AL5FE2                 AL5FE4:  RESTORED
TDB_SSOL2: GET
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
```

```
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   'Alan Dinsdale, SGTE Data for Pure Elements,
       Calphad Vol 15(1991) p 317-425,
       also in NPL Report DMA(A)195 Rev. August 1990'
   'Marion Seiersten, unpublished work (1989); Al-Fe'
   'Alan Dinsdale, SGTE Data for Pure Elements, NPL Report DMA(A)195
       September 1989'
 UNARY G0 PARAMETERS ARE MISSING
 BINARY L0 PARAMETERS ARE MISSING
 CHECK THE FILE MISSING.LIS FOR COMPLETE INFO
 -OK-
TDB_SSOL2: GO P-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ Calculate an equilibrium where BCC is ordered
POLY_3: S-C T=1300,P=1E5,N=1,X(AL)=.3
   ... the command in full is SET_CONDITION
POLY_3: C-E
   ... the command in full is COMPUTE_EQUILIBRIUM
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    45 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ List the equilibrium. Note that option N gives the
POLY_3: @@ constitution of the BCC phase and this shows that the
POLY_3: @@ site-fractions are different in the two sublattices,
POLY_3: @@ i.e. the BCC is ordered
POLY_3: L-E
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWNS/:  N
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL2

 Conditions:
 T=1300, P=1E5, N=1, X(AL)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1300.00 K (  1026.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.71874E+01
 Total Gibbs energy -8.63082E+04,  Enthalpy  1.26388E+04,  Volume  5.19721E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      3.0000E-01  1.7154E-01 3.1524E-05 -1.1203E+05 SER
 FE                      7.0000E-01  8.2846E-01 9.4433E-04 -7.5284E+04 SER

 B2_BCC                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.7187E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  8.28461E-01  AL  1.71539E-01
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  8.77450E-01  AL  1.22550E-01
 Sublattice  2,  Number of sites  5.0000E-01
 FE  5.22550E-01  AL  4.77450E-01
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Set axis
POLY_3: S-A-V 1 X(AL)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  1
Increment /.025/:  .025
POLY_3: S-A-V 2 T
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  500
Max value /1/:  2000
Increment /37.5/:  25
POLY_3: SAVE tcex16 Y
```

... the command in full is SAVE_WORKSPACES

```
 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.
```

POLY_3: **MAP**

```
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   5.230E-01  5.100E+02
  ** AL2FE
     B2_BCC
 Calculated..             2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   5.225E-01  5.000E+02
  ** AL2FE
     B2_BCC
 Calculated.            33  equilibria

 Phase region boundary   3 at:   5.865E-01  1.296E+03
  ** AL2FE
  ** AL5FE4
     B2_BCC

 Phase region boundary   4 at:   5.384E-01  1.296E+03
  ** AL5FE4
```

```
    B2_BCC
 Calculated.           10  equilibria

       :
       :
       :

 Phase region boundary  43 at:   6.423E-01  1.458E+03
    LIQUID
  ** AL5FE4
 Calculated.            8  equilibria
 Terminating at known equilibrium

 Phase region boundary  44 at:   6.423E-01  1.458E+03
    LIQUID
  ** AL5FE4
 Calculated.            3  equilibria
 Terminating at known equilibrium

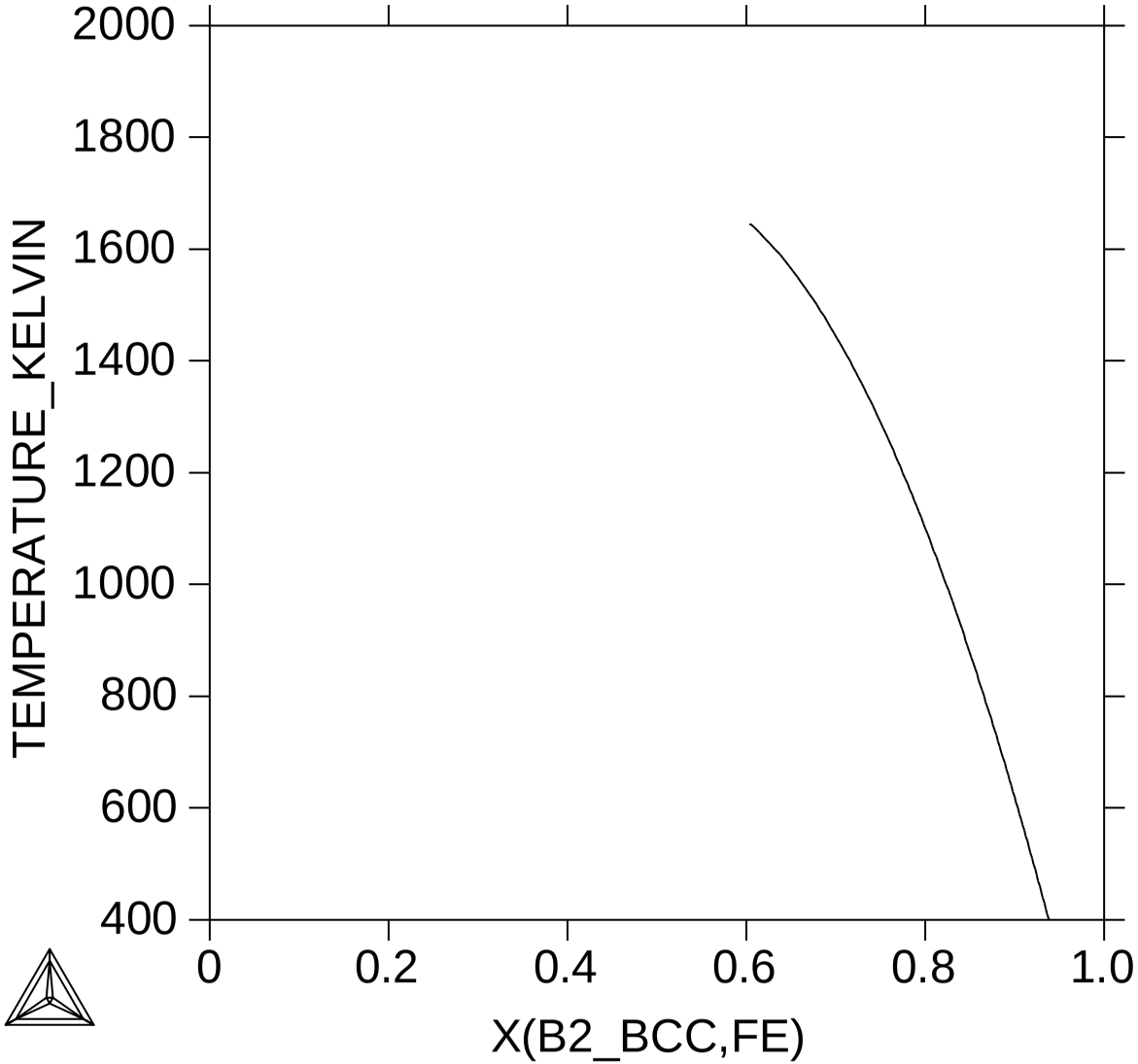
 Phase region boundary  45 at:   8.763E-01  9.397E+02
    LIQUID
  ** AL13FE4
 Calculated.           28  equilibria
 Terminating at known equilibrium

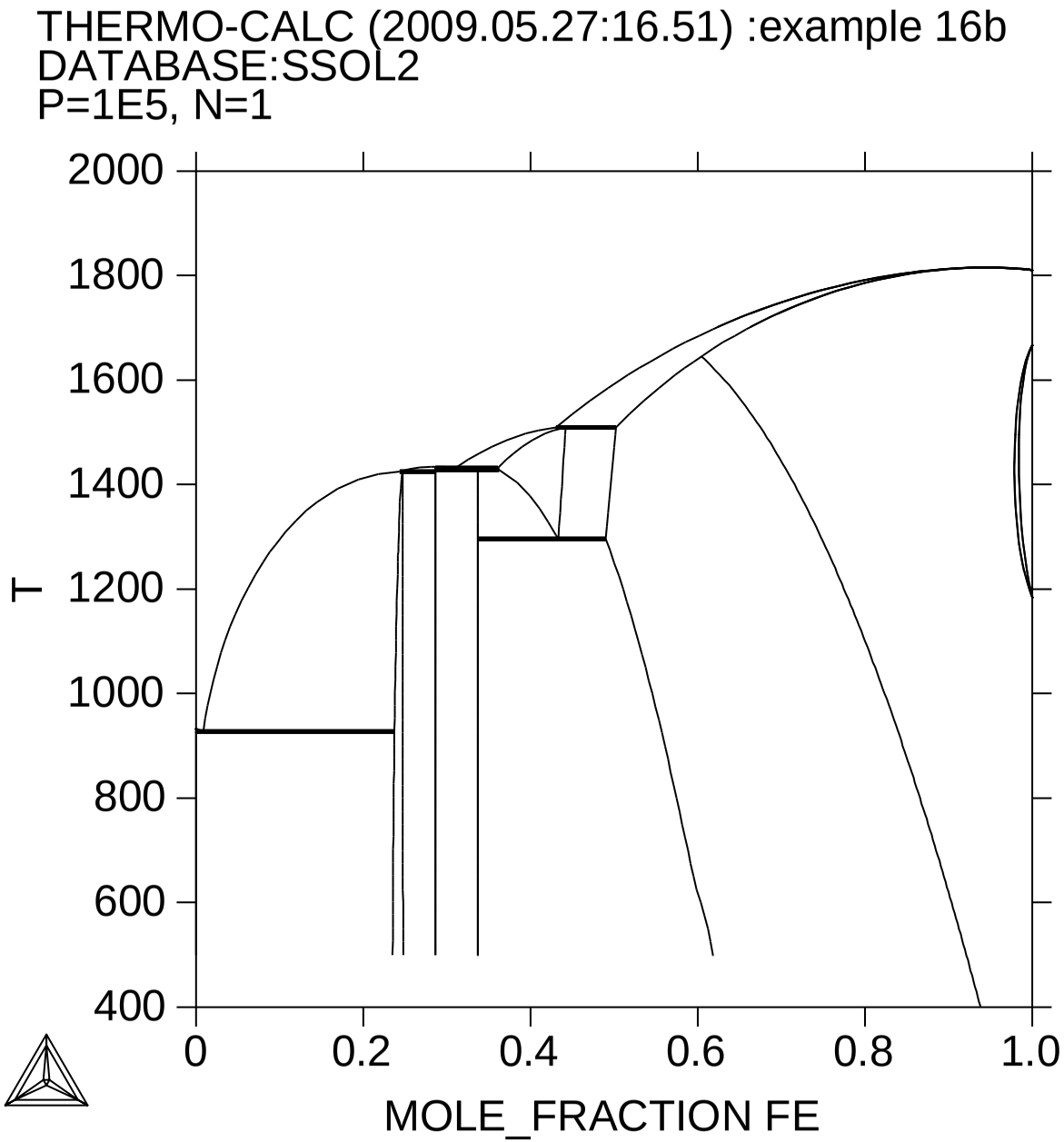
 Phase region boundary  46 at:   8.763E-01  9.397E+02
    LIQUID
  ** AL13FE4
 Calculated.            2  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex16.POLY3
 CPU time for mapping           4  seconds
POLY_3:
POLY_3: POST
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,,,,,,,
POST:
POST: S-D-A X M-F FE
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y T
   ... the command in full is SET_DIAGRAM_AXIS
POST: @@ Append the previous line for the 2nd order transition
POST: A-E-D Y TCEX16
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  1
POST: set-title example 16b
POST: PLOT
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
 CPU time           5  seconds
```

THERMO-CALC (2009.05.28:09.33) :example 16a
DATABASE:SSOL2
P=1E5, N=1., Y(B2_BCC,FE)-Y(B2_BCC,FE#2)=1.0001E-4;




THERMO-CALC (2009.05.27:16.51) :example 16b
DATABASE:SSOL2
P=1E5, N=1
2000
1800
1600
1400
1200
1000
800
600
400
T
0
0.2
0.4
0.6
0.8
1.0
MOLE_FRACTION FE

17

Calculation of pseudo-binary phase diagram in the CaO-SiO_2 system

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of the pseudo-binary system CaO-SiO2
SYS: @@ using the ionic database
SYS: @@
SYS: set-log ex17,,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: @@ This database can be used both for pseudobinary systems like
TDB_TCFE6: @@ the one in this case, CaO-SiO2, or for full ternary systems
TDB_TCFE6: @@ like Ca-Fe-O.
TDB_TCFE6: sw pion
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Ionic Solutions TDB v2

 VA                      /-  DEFINED
 LIQUID:L  REJECTED
TDB_PION: @@ Note that /- represent the electon.
TDB_PION: d-sys ca si o
   ... the command in full is DEFINE_SYSTEM
 CA                      SI                      O
   DEFINED
TDB_PION: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:  CONSTITUENT
 GAS:G       :O2:
  > This is the pure O2 gaseous phase
 IONIC_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 VA SIO2:
  > Ionic Liquid Solution: using the ionic two-sublattice model
 FCC_A1      :CA O SI:VA:
 BCC_A2      :CA O SI:VA:
 DIAMOND_FCC_A4 :O SI:
 OLIVINE     :CA+2:CA+2:SI+4:O-2:
 HALITE:I    :CA+2 VA:O-2:
 WOLLASTONITE :CA+2:SI+4:O-2:
 PSEUDO_WOLLASTONITE :CA+2:SI+4:O-2:
 RANKINITE   :CA+2:SI+4:O-2:
 HATRURITE   :CA+2:SI+4:O-2:
 LARNITE     :CA+2:SI+4:O-2:
 ALPHA_CA2SIO4 :CA+2:SI+4:O-2:
 ALPHA_PRIME_CA2SIO4 :CA+2:SI+4:O-2:
 QUARTZ      :SIO2:
 TRIDYMITE   :SIO2:
 CRISTOBALITE :SIO2:
 HCP_A3      :CA SI:VA:
 CBCC_A12    :SI:VA:
 CUB_A13     :SI:VA:
 CA2SI       :CA:SI:
 CASI        :CA:SI:
 CASI2       :CA:SI:
 CR3SI       :SI:SI:
 CRSI2       :SI:SI:
TDB_PION: @@ If we want to calculate a pseudobinary system
TDB_PION: @@ we must take away all phases and constituents that make it
TDB_PION: @@ possible for the phase to exist outside the composition line
TDB_PION: @@ from CaO to SiO2.
TDB_PION: @@ This means that for the IONIC_LIQ phase the constituent Va should
TDB_PION: @@ be suspended for systems with no degree of freedom with
TDB_PION: @@ respect to oxygen
TDB_PION: rej const
```

```
   ... the command in full is REJECT
PHASE: ion
SUBLATTICE NUMBER: 2
CONSTITUENT: va
 VA IN IONIC_LIQ:Y SUBLATTICE   2 REJECTED
CONSTITUENT:
TDB_PION: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
 GAS:G       :O2:
  > This is the pure O2 gaseous phase
 IONIC_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 SIO2:
  > Ionic Liquid Solution: using the ionic two-sublattice model
 FCC_A1      :CA O SI:VA:
 BCC_A2      :CA O SI:VA:
 DIAMOND_FCC_A4 :O SI:
 OLIVINE     :CA+2:CA+2:SI+4:O-2:
 HALITE:I    :CA+2 VA:O-2:
 WOLLASTONITE :CA+2:SI+4:O-2:
 PSEUDO_WOLLASTONITE :CA+2:SI+4:O-2:
 RANKINITE   :CA+2:SI+4:O-2:
 HATRURITE   :CA+2:SI+4:O-2:
 LARNITE     :CA+2:SI+4:O-2:
 ALPHA_CA2SIO4 :CA+2:SI+4:O-2:
 ALPHA_PRIME_CA2SIO4 :CA+2:SI+4:O-2:
 QUARTZ      :SIO2:
 TRIDYMITE   :SIO2:
 CRISTOBALITE :SIO2:
 HCP_A3      :CA SI:VA:
 CBCC_A12    :SI:VA:
 CUB_A13     :SI:VA:
 CA2SI       :CA:SI:
 CASI        :CA:SI:
 CASI2       :CA:SI:
 CR3SI       :SI:SI:
 CRSI2       :SI:SI:
TDB_PION: @?<Hit_return_to_continue>
TDB_PION: @@ The phase names may seem unfamiliar but this is due to the
TDB_PION: @@ attempt to create a general database. Thus lime (CaO) is
TDB_PION: @@ called HALITE which is the generic phase name for this structure.
TDB_PION: @@ HALITE is also the wudstite phase (FeO) and the periclase phase (MgO)
TDB_PION: @@ Note also that many phases are modelled with sublattices and
TDB_PION: @@ vacancies in order to allow for non-stoichiometry in higher
TDB_PION: @@ order system.
TDB_PION: @@ For simplicity we reject all phases except those we know
TDB_PION: @@ should be stable in this system.
TDB_PION: @@
TDB_PION: rej ph /all
   ... the command in full is REJECT
 GAS:G                  IONIC_LIQ:Y            FCC_A1
 BCC_A2                 DIAMOND_FCC_A4         OLIVINE
 HALITE:I               WOLLASTONITE           PSEUDO_WOLLASTONITE
 RANKINITE              HATRURITE              LARNITE
 ALPHA_CA2SIO4          ALPHA_PRIME_CA2SIO4    QUARTZ
 TRIDYMITE              CRISTOBALITE           HCP_A3
 CBCC_A12               CUB_A13                CA2SI
 CASI                   CASI2                  CR3SI
 CRSI2  REJECTED
TDB_PION: rest ph ion alpha_ca2sio4 alpha_prime crist halite hatru
   ... the command in full is RESTORE
 IONIC_LIQ:Y            ALPHA_CA2SIO4          ALPHA_PRIME_CA2SIO4
 CRISTOBALITE           HALITE:I               HATRURITE
   RESTORED
TDB_PION: rest ph larn oliv pseudo quartz rank tri wolla
   ... the command in full is RESTORE
 LARNITE                OLIVINE                PSEUDO_WOLLASTONITE
 QUARTZ                 RANKINITE              TRIDYMITE
 WOLLASTONITE  RESTORED
TDB_PION: @@ To avoid complications we should also reject the Si+4 in the
TDB_PION: @@ first sublattice in the liquid phase. When there is oxygen present
TDB_PION: @@ all Si will form SiO2 or SiO4/-4. The Si+4 ion is needed only
TDB_PION: @@ for the liquid in systems without oxygen.
TDB_PION: rej const ion
   ... the command in full is REJECT
```

```
SUBLATTICE NUMBER: 1
CONSTITUENT: si+4
 SI+4 IN IONIC_LIQ:Y SUBLATTICE   1 REJECTED
CONSTITUENT:
TDB_PION: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/:
 IONIC_LIQ:Y :CA+2:O-2 SIO4-4 SIO2:
  > Ionic Liquid Solution: using the ionic two-sublattice model
 OLIVINE     :CA+2:CA+2:SI+4:O-2:
 HALITE:I    :CA+2 VA:O-2:
 WOLLASTONITE :CA+2:SI+4:O-2:
 PSEUDO_WOLLASTONITE :CA+2:SI+4:O-2:
 RANKINITE   :CA+2:SI+4:O-2:
 HATRURITE   :CA+2:SI+4:O-2:
 LARNITE     :CA+2:SI+4:O-2:
 ALPHA_CA2SIO4 :CA+2:SI+4:O-2:
 ALPHA_PRIME_CA2SIO4 :CA+2:SI+4:O-2:
 QUARTZ      :SIO2:
 TRIDYMITE   :SIO2:
 CRISTOBALITE :SIO2:
TDB_PION: @?<Hit_return_to_continue>
TDB_PION:
TDB_PION: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, Private Communication, (liquid and solid Al2O3,CaO,MgO). '
  'M. Hillert, B. Sundman and X. Wang, Calphad, 15 (1991), 53-58,
      [Reassessm. CaO-SiO2 (rank, ps, alpha, ion)]. '
  'T.I. Barry (1987): NPL, UK, Unpublished research (liquid and solid SiO2). '
  'M. Hillert, B. Sundman and X. Wang (1990): Metall Trans B, 21B, 303-312
      (CaO-SiO2). '
  'W. Huang, M. Hillert and X. Wang (1995): Metall Mater Trans A, 26A, 2293
      -231 (CaO-MgO-SiO2). '
 -OK-
TDB_PION:
TDB_PION: @@ There is a miscibility gap in the ionic liquid close to SiO2.
TDB_PION: @@ In this database two composition sets will be created automatically
TDB_PION: @@ and one will have SiO2 as major constituent
TDB_PION:
TDB_PION: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ Define more convenient components than the elements
POLY_3: list-stat
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 CA                      ENTERED   SER
 O                       ENTERED   SER
 SI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 WOLLASTONITE            ENTERED    0.00000000E+00  0.00000000E+00
 TRIDYMITE               ENTERED    0.00000000E+00  0.00000000E+00
 RANKINITE               ENTERED    0.00000000E+00  0.00000000E+00
 QUARTZ                  ENTERED    0.00000000E+00  0.00000000E+00
 PSEUDO_WOLLASTONITE     ENTERED    0.00000000E+00  0.00000000E+00
 OLIVINE                 ENTERED    0.00000000E+00  0.00000000E+00
 LARNITE                 ENTERED    0.00000000E+00  0.00000000E+00
 HATRURITE               ENTERED    0.00000000E+00  0.00000000E+00
 HALITE                  ENTERED    0.00000000E+00  0.00000000E+00
```

```
 CRISTOBALITE            ENTERED    0.00000000E+00  0.00000000E+00
 ALPHA_PRIME_CA2SIO4     ENTERED    0.00000000E+00  0.00000000E+00
 ALPHA_CA2SIO4           ENTERED    0.00000000E+00  0.00000000E+00
 IONIC_LIQ#3             ENTERED    0.00000000E+00  0.00000000E+00
 IONIC_LIQ#2             ENTERED    0.00000000E+00  0.00000000E+00
 IONIC_LIQ#1             ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 CA     ENTERED    O      ENTERED    SI     ENTERED    SIO4-4 ENTERED
 CA+2   ENTERED    O-2    ENTERED    SI+4   ENTERED    VA     ENTERED
 CAO    ENTERED    O2     ENTERED    SIO2   ENTERED
POLY_3: def-com cao sio2 o
   ... the command in full is DEFINE_COMPONENTS
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 CAO                     ENTERED   SER
 SIO2                    ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 WOLLASTONITE            ENTERED    0.00000000E+00  0.00000000E+00
 TRIDYMITE               ENTERED    0.00000000E+00  0.00000000E+00
 RANKINITE               ENTERED    0.00000000E+00  0.00000000E+00
 QUARTZ                  ENTERED    0.00000000E+00  0.00000000E+00
 PSEUDO_WOLLASTONITE     ENTERED    0.00000000E+00  0.00000000E+00
 OLIVINE                 ENTERED    0.00000000E+00  0.00000000E+00
 LARNITE                 ENTERED    0.00000000E+00  0.00000000E+00
 HATRURITE               ENTERED    0.00000000E+00  0.00000000E+00
 HALITE                  ENTERED    0.00000000E+00  0.00000000E+00
 CRISTOBALITE            ENTERED    0.00000000E+00  0.00000000E+00
 ALPHA_PRIME_CA2SIO4     ENTERED    0.00000000E+00  0.00000000E+00
 ALPHA_CA2SIO4           ENTERED    0.00000000E+00  0.00000000E+00
 IONIC_LIQ#3             ENTERED    0.00000000E+00  0.00000000E+00
 IONIC_LIQ#2             ENTERED    0.00000000E+00  0.00000000E+00
 IONIC_LIQ#1             ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 CA     ENTERED    O      ENTERED    SI     ENTERED    SIO4-4 ENTERED
 CA+2   ENTERED    O-2    ENTERED    SI+4   ENTERED    VA     ENTERED
 CAO    ENTERED    O2     ENTERED    SIO2   ENTERED
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-c t=2000,p=1e5,n=1,w(sio2)=.9
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=2000, P=1E5, N=1, W(SIO2)=0.9
 DEGREES OF FREEDOM 1
POLY_3: @@ There is one degree of freedom due to the oxygen. As the oxygen content
POLY_3: @@ is determined by the Ca/Si ration there is no possibility to vary
POLY_3: @@ the oxygen content in this system independently. Thus the
POLY_3: @@ oxygen potential can be set to any value (larger than zero).
POLY_3: s-c ac(o)=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         2021  grid points in            0  s
    46 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: @@ Option N is used to include information on the
POLY_3: @@ constitution of the phases.
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  n
 Output from POLY-3, equilibrium =     1, label A0  , database: PION

 Conditions:
 T=2000, P=1E5, N=1, W(SIO2)=0.9, AC(O)=1
 DEGREES OF FREEDOM 0
```

```
 Temperature   2000.00 K (  1726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.96571E+01
 Total Gibbs energy -1.10541E+06,  Enthalpy -7.53274E+05,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CAO                     1.0638E-01  1.0000E-01 6.4224E-25 -9.2632E+05 SER
 SIO2                    8.9362E-01  9.0000E-01 3.7467E-30 -1.1267E+06 SER
 O                       0.0000E+00  1.0668E-18 1.0000E+00  0.0000E+00 SER

 IONIC_LIQ#2                 Status ENTERED     Driving force  0.0000E+00
 Moles 6.7245E-01, Mass 4.0314E+01, Volume fraction 0.0000E+00  Mass fractions:
 SIO2  9.69163E-01  CAO   3.08366E-02  O     0.00000E+00
 Constitution:
 Sublattice  1,  Number of sites  6.8156E-02
 CA+2    1.00000E+00
 Sublattice  2,  Number of sites  2.0000E+00
 SIO2    9.82793E-01  SIO4-4  1.68709E-02  O-2     3.36172E-04

 IONIC_LIQ#3                 Status ENTERED     Driving force  0.0000E+00
 Moles 3.2755E-01, Mass 1.9343E+01, Volume fraction 0.0000E+00  Mass fractions:
 SIO2  7.55851E-01  CAO   2.44149E-01  O     0.00000E+00
 Constitution:
 Sublattice  1,  Number of sites  6.9176E-01
 CA+2    1.00000E+00
 Sublattice  2,  Number of sites  2.0000E+00
 SIO2    8.26780E-01  SIO4-4  1.72662E-01  O-2     5.57209E-04
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The result shows the expected miscibility gap. However, in some
POLY_3: @@ cases the first calculation may fail. In such cases try to simplify the
POLY_3: @@ calculation by suspending all phases but the important ones.
POLY_3: @@ Save the results so far on file
POLY_3: save tcex17 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ Set the axis
POLY_3: s-a-v 1 w(sio2)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  1
Increment /.025/:  .025
POLY_3: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  1500
Max value /1/:  3500
Increment /50/:  20
POLY_3: save tcex17 Y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
```

```
 Generating start point  10
 Working hard
  ..
  ..
  ..
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   1.765E-01  1.510E+03
  ** ALPHA_PRIME_CA2SIO4
     HALITE
 *** Buffer saved on file: tcex17.POLY3
 Calculated..            2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   1.765E-01  1.500E+03
  ** ALPHA_PRIME_CA2SIO4
     HALITE
 Calculated.             3  equilibria

 Phase region boundary   3 at:   1.765E-01  1.525E+03
  ** ALPHA_PRIME_CA2SIO4
     HALITE
  ** HATRURITE

 Phase region boundary   4 at:   1.327E-01  1.525E+03
     HALITE
  ** HATRURITE
 Calculated.            46  equilibria
  ..
  ..
  ..
 Phase region boundary  60 at:   8.337E-01  1.812E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated.             9  equilibria
 Terminating at known equilibrium

 Phase region boundary  61 at:   9.950E-01  1.978E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated             7  equilibria

 Phase region boundary  62 at:   9.950E-01  1.978E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated.             2  equilibria
 Terminating at known equilibrium

 Phase region boundary  63 at:   9.950E-01  1.978E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated            20  equilibria
 *** BUFFER SAVED ON FILE: tcex17.POLY3
 CPU time for mapping           6  seconds
POLY_3:
POLY_3: post

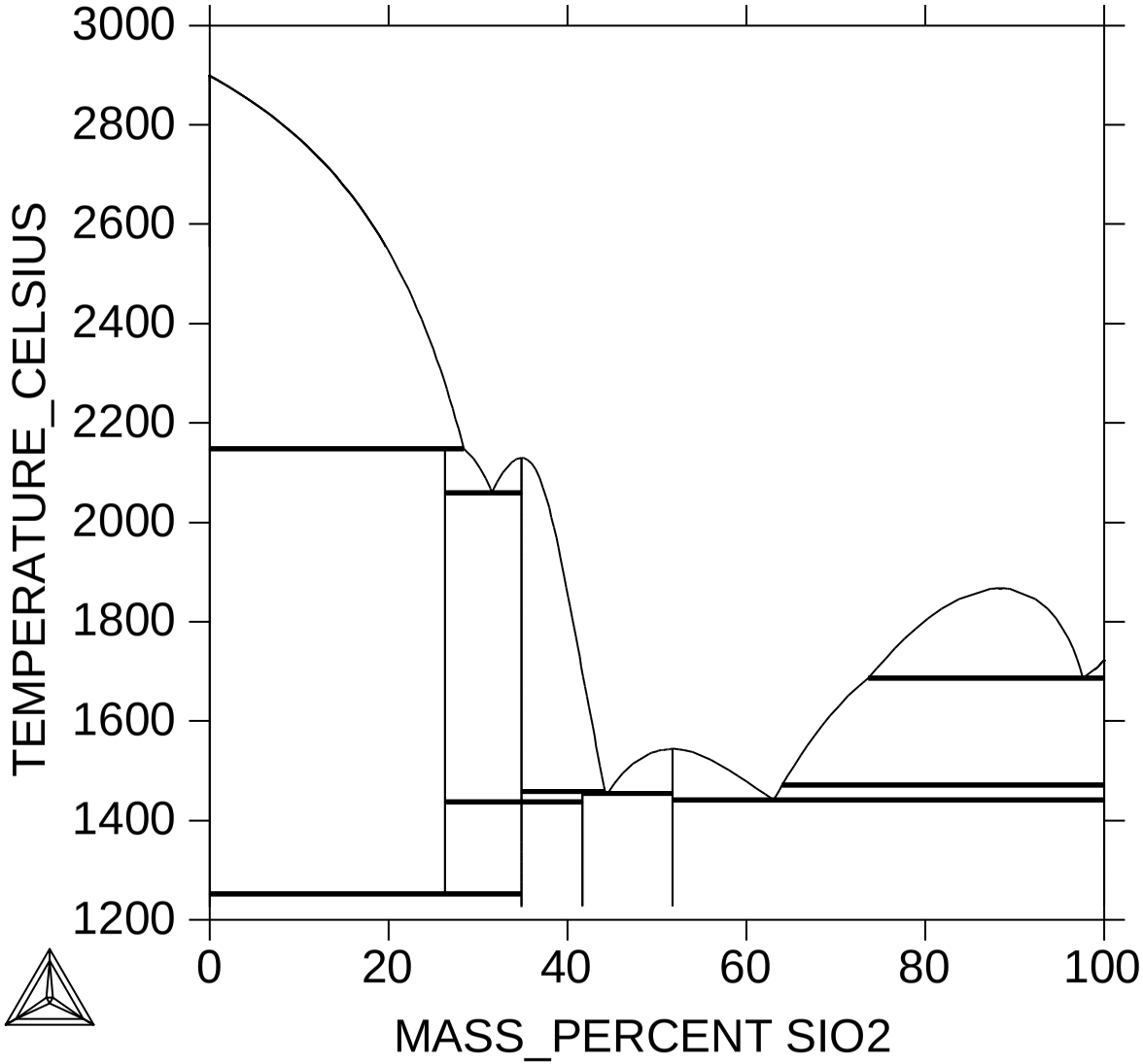
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

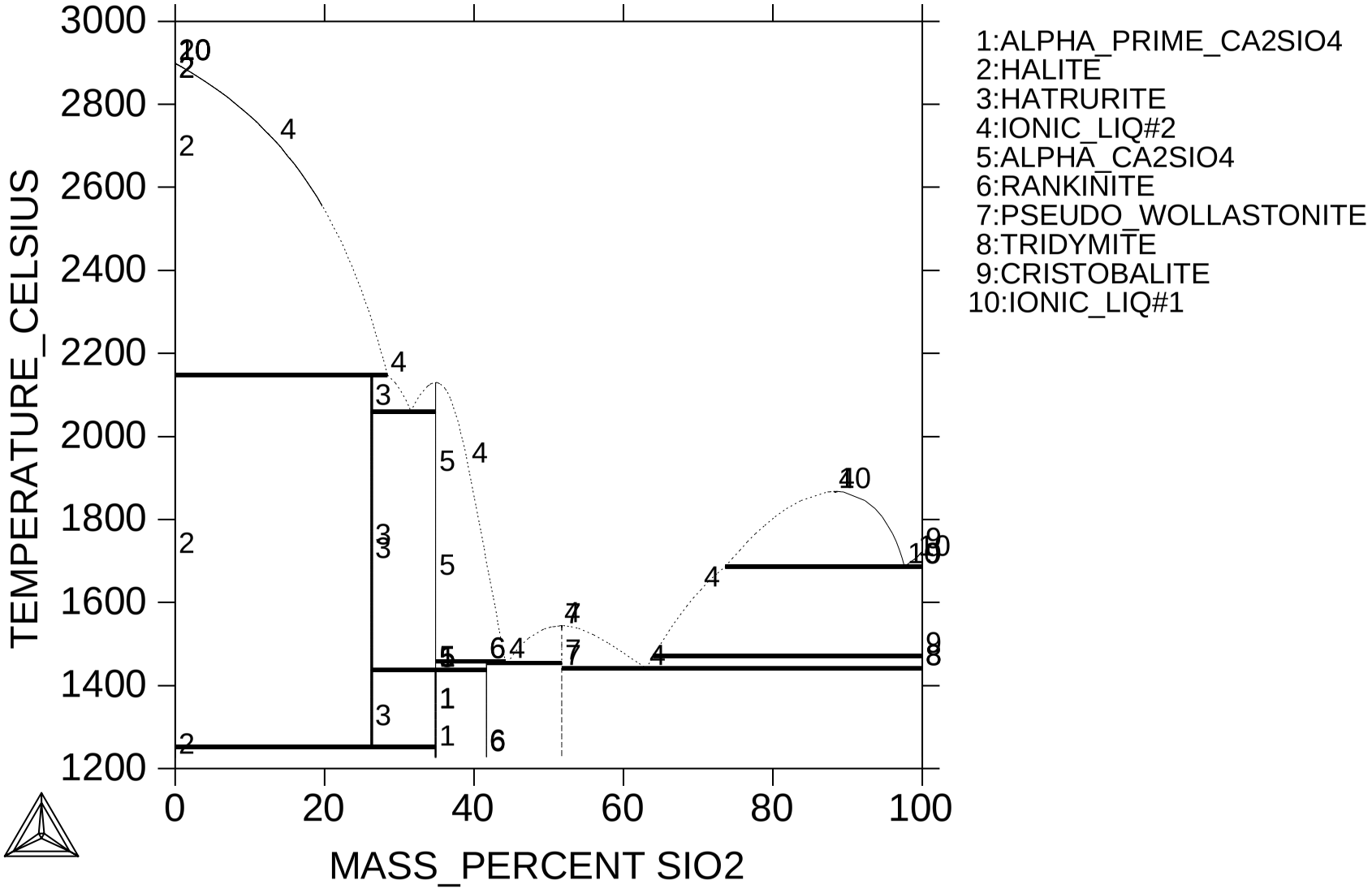
POST: s-d-a x w-p sio2
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 17a
```

```
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Indentify the phases with labels
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /A/:  f
POST: @@ Set font size to smaller to make room for all labels
POST: set-font
 CURRENT FONT: Cartographic Roman
SELECT FONTNUMBER /1/:
 NEW FONT: Cartographic Roman
FONT SIZE /.3400000036/:  .25
POST: set-title example 17b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time            6  seconds
```

THERMO-CALC (2009.04.15:03.02) :example 17a
DATABASE:PION
P=1E5, N=1, AC(O)=1;



THERMO-CALC (2009.04.15:03.02) :example 17b
DATABASE:PION
P=1E5, N=1, AC(O)=1;



18

Calculation of the A_3 temperature of a steel and the influence of each alloying element on this temperature

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ A3 temperature is the temperature where ferrite starts to form from
SYS: @@ austenite. One can easily read A3 from Fe-C phase diagram. But for
SYS: @@ complex multicomponent steels, no simple diagram can be used.
SYS: @@ This example shows how to calculate the A3 temperature of a steel.
SYS: @@ Using the facility in POLY, it is easy to find out the influence
SYS: @@ of each alloying element on A3 temperature. This information is
SYS: @@ useful if one wants to modify the compositions of a steel but keep
SYS: @@ A3 unchanged.
SYS: @@
SYS: set-log ex18,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/:  tcfe6
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: cr 1.5 mn .5 c .3 si .3 nb .1
Next alloying element:
Temperature (C) /1000/:  1100
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NB  DEFINED

 This database has following phases for the defined system

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 KSI_CARBIDE             A1_KAPPA                KAPPA
 Z_PHASE                 FE4N_LP1                FECN_CHI
 SIGMA                   MU_PHASE                CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   AL4C3                   FE8SI2C
 SIC

Reject phase(s) /NONE/:  ?
 Reject phase(s)

  This is a question generated by the database allowing the user to select
```

the phases. Normally, all phases should be included and the user just presses <RETURN>.

If a phase is to be rejected, the name of the phase must be supplied. Several phase names can be specified in one line.

It is possible to reject all phase by giving an asterisk "*". If the number of phases to be included is much smaller than the total number of phases, it may be convenient to first reject all phases and then restore just those that should be included.

Note: This question will be repeated until the user press <RETURN> after rejected all undesired phases or an asterisk "*".

```
Reject phase(s) /NONE/: *
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 KSI_CARBIDE             A1_KAPPA                KAPPA
 Z_PHASE                 FE4N_LP1                FECN_CHI
 SIGMA                   MU_PHASE                CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   AL4C3                   FE8SI2C
 SIC  REJECTED
Restore phase(s):: liq fcc bcc hcp gra cem m23 m7
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  GRAPHITE                CEMENTITE
 M23C6                   M7C3  RESTORED
Restore phase(s): /NONE/:

 ....................................................

    The following phases are retained in this system:

 LIQUID:L                 BCC_A2                   FCC_A1
 HCP_A3                   GRAPHITE                 CEMENTITE
 M23C6                    M7C3

 ....................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'B.-J. Lee, estimated parameter 1999'
  'J. Grobner, H.L. Lukas and F. Aldinger, Calphad, 20 (1996), 247-254; Si-C
      and Al-Si-C'
                    :
                    :
                    :
  'K. Frisk, Calphad, 17 (1993), 335-349; Cr-Mn-N'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'C. Qiu, Metall. Trans. A, 24A (1993), 2393-2409; Cr-Fe-Mn-N'
  'W. Huang, Z. fur Metallkde., 81 (1990), 397-404; TRITA-MAC 390 (1989);
      FE-NB, C-FE-NB'
  'P. Villars and L.D. Calvert (1985). Pearson´s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
```

```
 -OK-
Should any phase have a miscibility gap check? /N/:  N
 Using global minimization procedure
 Calculated        10004  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3:
POLY_3:
POLY_3: @@ In the TCFE database the number of phases is very large.
POLY_3: @@ It is strongly recommended that one rejects all phases
POLY_3: @@ that one knows should not be stable
POLY_3:
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
    P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1373.15 K (  1100.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50375E+01
 Total Gibbs energy -7.21999E+04,  Enthalpy  4.05686E+04,  Volume  7.32058E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3747E-02  3.0000E-03 1.0740E-02 -5.1763E+04 SER
 CR                      1.5877E-02  1.5000E-02 1.3123E-04 -1.0205E+05 SER
 FE                      9.5890E-01  9.7300E-01 2.0390E-03 -7.0732E+04 SER
 MN                      5.0091E-03  5.0000E-03 4.2846E-06 -1.4112E+05 SER
 NB                      5.9240E-04  1.0000E-03 1.3310E-07 -1.8076E+05 SER
 SI                      5.8788E-03  3.0000E-03 1.1131E-08 -2.0909E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.9900E-01, Mass 5.4984E+01, Volume fraction 9.9904E-01  Mass fractions:
 FE  9.73932E-01  MN  5.00479E-03  C   2.89608E-03
 CR  1.50122E-02  SI  3.00290E-03  NB  1.51584E-04

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0011E-03, Mass 5.3091E-02, Volume fraction 9.5720E-04  Mass fractions:
 NB  8.79676E-01  FE  7.33072E-03  MN  3.71964E-05
 C   1.10624E-01  CR  2.33143E-03  SI  1.24275E-09
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Two FCC phases are stable, one with mainly Fe and
POLY_3: @@ one with mainly Nb and C, which is the NbC carbide.
POLY_3: @@ The second fcc is called FCC#2. The digit after # is
POLY_3: @@ called composition set but can be ignored if it is unity.
POLY_3:
POLY_3: li-st
   ... the command in full is LIST_STATUS
Option /CPS/:  CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 NB                      ENTERED   SER
 SI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FCC_A1#2                ENTERED    0.00000000E+00  1.00105304E-03
 FCC_A1#1                ENTERED    0.00000000E+00  9.98998937E-01
 BCC_A2                  ENTERED   -1.87737409E-02  0.00000000E+00
 LIQUID                  ENTERED   -2.06845888E-01  0.00000000E+00
 HCP_A3#1                ENTERED   -3.23829327E-01  0.00000000E+00
 HCP_A3#2                ENTERED   -3.23829327E-01  0.00000000E+00
 M23C6                   ENTERED   -3.97577114E-01  0.00000000E+00
 CEMENTITE               ENTERED   -4.57991155E-01  0.00000000E+00
 M7C3                    ENTERED   -6.05087890E-01  0.00000000E+00
 GRAPHITE                ENTERED   -2.50468908E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
```

```
 C  ENTERED    FE ENTERED    NB ENTERED    VA ENTERED
 CR ENTERED    MN ENTERED    SI ENTERED
POLY_3:
POLY_3: @@ Fcc appears twice on the list above. The HCP phase also has
POLY_3: @@ two composition sets.
POLY_3:
POLY_3: @@ This result looks reasonable, save it on a file
POLY_3: save tcex18 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: @@ Now calculate when bcc (ferrite) begins to form
POLY_3: @@ using the COMPUTE-TRANSITION command
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc
 You must release one of these conditions
 T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
 P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/:  t
 Testing POLY result by global minimization procedure
 Calculated        10004  grid points in           0  s
To form BCC the condition is set to T=1071.60881565
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ We may expect BCC to form at a lower temperature, because sometimes
POLY_3: @@ a higer temperature is found as there is a delta-ferrite stable
POLY_3: @@ at high temperatures.
POLY_3: @@
POLY_3: @@ Calculate again the equilibrium at lower temperature.  You can
POLY_3: @@ do this by just a SET-COND T=... command but then the temperature must
POLY_3: @@ be given in Kelvin.  You can use the DEF-MAT command to do this
POLY_3: @@ in Celsius
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
Same elements as before? /Y/:  Y
Mass (weight) percent of C /.3/:  .3
Mass (weight) percent of CR /1.5/:  1.5
Mass (weight) percent of MN /.5/:  .5
Mass (weight) percent of NB /.1/:  .1
Mass (weight) percent of SI /.3/:  .3
Temperature (C) /798/:  800
 Using global minimization procedure
 Calculated        10004  grid points in           1  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
    P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1073.15 K (   800.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50375E+01
 Total Gibbs energy -4.87895E+04,  Enthalpy  3.03117E+04,  Volume  7.17692E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3747E-02  3.0000E-03 4.4068E-02 -2.7857E+04 SER
 CR                      1.5877E-02  1.5000E-02 3.5554E-04 -7.0863E+04 SER
 FE                      9.5890E-01  9.7300E-01 4.8677E-03 -4.7515E+04 SER
 MN                      5.0091E-03  5.0000E-03 8.2064E-06 -1.0449E+05 SER
 NB                      5.9240E-04  1.0000E-03 2.9934E-09 -1.7512E+05 SER
 SI                      5.8788E-03  3.0000E-03 8.9756E-10 -1.8587E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.9870E-01, Mass 5.4971E+01, Volume fraction 9.9878E-01  Mass fractions:
 FE  9.74156E-01  MN  5.00593E-03  C   2.86369E-03
 CR  1.49685E-02  SI  3.00361E-03  NB  2.74704E-06

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.2984E-03, Mass 6.6134E-02, Volume fraction 1.2211E-03  Mass fractions:
```

```
 NB  8.29930E-01  CR  4.11711E-02  MN  7.37925E-05
 C   1.16301E-01  FE  1.25236E-02  SI  1.74994E-10
POLY_3:
POLY_3: @@ Try a slightly different COMPUTE-TRANSITION command.
POLY_3: @@ This finds the first phase change in the specified direction.
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: any
 You must release one of these conditions
 T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
 P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/:  t
Estimated change (with sign) /1/:  ?
 Estimated change (with sign)

  A given varying direction sign and an estimated change of the released
  condition, in this case X(FE), must be given here: a negative sign means
  at a lower value of the released condition any new phase is to be found,
  and a positive sign at a higher value; an estimated change of the released
  condition implies where any new phase is expected (but it is only estimated
  value, so any value within its reasonable scale would be enough).

  For instance, if a combination of -.02 is input, the following message may
  come up (after a successful calculation):
    To form BCC_A2#1 the condition is set to X(FE)=.493708756187

  This calculated value will then be assign as the parameter of that removed
  condition, in this case, the X(FE) variable. So the following message will
  be shown on the screen, if the LIST_CONDITIONS command is typed:
    P=100000, T=800, N=1, X(FE)=4.93708756E-1
    DEGREES OF FREEDOM 0

Estimated change (with sign) /1/:  -1
 Testing POLY result by global minimization procedure
 Calculated        10004  grid points in           0  s
To form BCC_A2#1 the condition is set to T=1071.60881565
POLY_3: show t
   ... the command in full is SHOW_VALUE
 T=1071.6088
POLY_3: @@ The transition temperature to form BCC is the same.
POLY_3: @@ If we want it in Celsius enter a function for that.
POLY_3: enter fun tc=t-273;
   ... the command in full is ENTER_SYMBOL
POLY_3: show tc
   ... the command in full is SHOW_VALUE
 TC=798.60882
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ This is the minimum temperature for hardening because below this
POLY_3: @@ temperature ferrite will form from austenite. Check how a small
POLY_3: @@ change of the composition can change this temperature. We must
POLY_3: @@ then set bcc as fix and release the condition on the temperature.
POLY_3: c-st p bcc=fix 0
   ... the command in full is CHANGE_STATUS
POLY_3: s-c t=none
   ... the command in full is SET_CONDITION
POLY_3: @@ The change of the calculated temperature for a small change of
POLY_3: @@ the amount of a component can be calculated as a derivative
POLY_3: @@ using the dot "." between the calculated variable and the condition.
POLY_3: sh t.w(mn)
   ... the command in full is SHOW_VALUE
 T.W(MN)=-2592.1917
POLY_3: sh t.w(cr)
   ... the command in full is SHOW_VALUE
 T.W(CR)=-781.45507
POLY_3: sh t.w(nb)
   ... the command in full is SHOW_VALUE
 T.W(NB)=3005.9537
POLY_3: sh t.w(c)
   ... the command in full is SHOW_VALUE
 T.W(C)=-21796.295
POLY_3: sh t.w(si)
```

```
   ... the command in full is SHOW_VALUE
 T.W(SI)=2990.1116
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ A negative value means the temperature will decrease if the
POLY_3: @@ amount is increased. Check for Mn
POLY_3: s-c w(mn)
   ... the command in full is SET_CONDITION
Value /.005/:  .01
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated        10004  grid points in           0  s
     9 ITS,  CPU TIME USED   0 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1058.9661
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The temperature decreased from 1072 to 1059 i.e. 13 degrees.
POLY_3: @@ According to the derivatives calculated above, one could increase
POLY_3: @@ the temperature with the same amount by increasing the amount of Si
POLY_3: @@ 2592/2990=0.8669 times of the change in Mn i.e. from 0.3 to 0.733 %
POLY_3: s-c w(si)
   ... the command in full is SET_CONDITION
Value /.003/:  .00733
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated        10004  grid points in           0  s
    10 ITS,  CPU TIME USED   1 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1070.73
POLY_3: @@ The facility to calculate these derivatives is a powerful feature
POLY_3: @@ in order to find the best way to obtain a certain property of a material.
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3: CPU time           4  seconds
```

19

Mapping of univariant equilibria with the liquid in Al-Cu-Si

Part A. Step-by-step calculation

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS: @@    Part A: step-by-step calculation
SYS: @@
SYS: set-log ex19a,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw USER tcex19_cost2
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
TDB_USER: d-sys
   ... the command in full is DEFINE_SYSTEM
ELEMENTS: cu al si
 CU                      AL                      SI
   DEFINED
TDB_USER: l-s c
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :AL CU SI:
 ALCE_AMORPHOUS :AL:
 ALCUZN_T    :AL:CU VA:
 ALCU_DELTA  :AL:CU:
 ALCU_EPSILON :AL CU:CU:
 ALCU_ETA    :AL CU:CU:
 ALCU_PRIME  :AL:CU:
 ALCU_THETA  :AL:AL CU:
 ALCU_ZETA   :AL:CU:
 ALLI        :AL:VA:
 ALMO        :AL:AL:
 ALM_D019    :AL:AL:
 ALND_AMORPHOUS :AL:
 ALTI        :AL:AL:
 BCC_A2      :AL CU SI:VA:
 BCC_B2      :AL CU SI:AL CU SI:VA:
 BCT_A5      :AL:
 CBCC_A12    :AL SI:VA:
 CR3SI_A15   :SI:AL SI:
 CRSI2       :SI:SI:
 CU19SI6_ETA :CU:SI:
 CU33SI7_DELTA :CU:SI:
 CU4SI_EPSILON :CU:SI:
 CU56SI11_GAMMA :CU:SI:
 CU6Y        :CU:CU2:
 CUB_A13     :AL SI:VA:
 CUB_A15     :SI:AL SI:
 DIAMOND_A4  :AL SI:
 FCC_A1      :AL CU SI:VA:
 GAMMA_D83   :AL:AL CU:CU:
 GAMMA_H     :AL:AL CU:CU:
 HCP_A3      :AL CU SI:VA:
 HCP_ZN      :AL CU SI:VA:
 LAVES_C14   :AL CU:AL CU:
 LAVES_C15   :AL CU SI:AL CU SI:
 LAVES_C36   :AL CU:AL CU:
 SIV3        :SI:SI:
TDB_USER: get
   ... the command in full is GET_DATA
```

```
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 Reference REF1       missing
 Reference REF1       missing
 Reference REF1       missing
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1300,p=101325,n=1
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1300, P=1.01325E5, N=1
 DEGREES OF FREEDOM 2
POLY_3: s-c x(si)=.25,x(al)=.2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        16220  grid points in            1  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  vwcs
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1300, P=1.01325E5, N=1, X(SI)=0.25, X(AL)=0.2
 DEGREES OF FREEDOM 0

 Temperature   1300.00 K (  1026.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.73679E+01
 Total Gibbs energy -8.02595E+04,  Enthalpy  3.22931E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      2.0000E-01  1.1393E-01 5.1836E-05 -1.0666E+05 SER
 CU                      5.5000E-01  7.3785E-01 4.1349E-04 -8.4211E+04 SER
 SI                      2.5000E-01  1.4823E-01 9.3957E-03 -5.0450E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.7368E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  7.37847E-01  SI  1.48228E-01  AL  1.13925E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ we want to calculate the monovariant lines with liquid. Select
POLY_3: @@ two compositions and the temperature as axis
POLY_3: s-a-v 1 x(al)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  1
Increment /.025/:  .01
POLY_3: s-a-v 2 x(si)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  1
Increment /.025/:  .01
POLY_3: s-a-v 3 t 500 2000 25
   ... the command in full is SET_AXIS_VARIABLE
```

```
POLY_3: @@Set liquid as "present", otherwise all monovariant lines will be calculated.
POLY_3: @@ Previously, this was done by 'SPECIAL_OPTIONS'. In version S, it is
POLY_3: @@ regrouped into 'ADVANCED_OPTIONS'.
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  ?
 EQUILIBRIUM_CALCUL       OUTPUT_FILE_FOR_SHOW     STABILITY_CHECK
 GLOBAL_MINIMIZATION      PARAEQUILIBRIUM          STEP_AND_MAP
 LIST_PHASE_ADDITION      PHASE_ADDITION           T-ZERO TEMPERATURE
 MAJOR_CONSTITUENTS       PRESENT_PHASE            TOGGLE_ALTERNATE_MODE
 NEW_COMPOSITION_SET      SHOW_FOR_T=
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liquid
POLY_3:
POLY_3: save tcex19a1 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   8.426E-02  2.500E-01  1.182E+03
     LIQUID
  ** BCC_B2
  ** DIAMOND_A4
 *** Buffer saved on file: tcex19a1.POLY3
 CALCULATED    35 EQUILIBRIA

 Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
     LIQUID
     ALCU_EPSILON
  ** BCC_B2
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
     LIQUID
  ** ALCU_EPSILON
  ** BCC_B2
 Terminating at diagram limit
 CALCULATED    18 EQUILIBRIA

 Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4
 CALCULATED    20 EQUILIBRIA

       :
       :
       :

 Phase region boundary   2 at:   8.426E-02  2.500E-01  1.182E+03
     LIQUID
  ** BCC_B2
  ** DIAMOND_A4
 CALCULATED     8 EQUILIBRIA

 Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
     LIQUID
  ** BCC_B2
     CU19SI6_ETA
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
     LIQUID
  ** BCC_B2
  ** CU19SI6_ETA
 Terminating at diagram limit
```

```
 CALCULATED    12 EQUILIBRIA

 Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
     LIQUID
  ** CU19SI6_ETA
  ** DIAMOND_A4
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE: tcex19a1.POLY3
 CPU time for mapping           1  seconds
POLY_3:
POLY_3: @@ The monovariant line FCC/BCC/LIQ in the Cu corner is not connected,
POLY_3: @@ so add a start point for that. This is different from a MAP with
POLY_3: @@ two axes, where all connected or non-connected lines can be found
POLY_3: @@ automatically.
POLY_3: read tcex19a1
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c x(al)=.1 x(si)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        16220  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3:
POLY_3: map
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.390E-02  1.000E-01  1.285E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED    18 EQUILIBRIA

 Phase region boundary   2 at:   4.390E-02  1.000E-01  1.285E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE: tcex19a1.POLY3
 CPU time for mapping           0  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: @@ we want the liquid compositions only
POST: s-d-a x x(liq,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liq,si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,
POST:
POST:
POST: set-title example 19Aa
POST: plot
```

```
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Make it triangular and scale the axis
POST: s-d-t
   ... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM  (Y OR N) /N/:  y,,,,,,
POST: s-sc y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-sc x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: @@ Plot the phases stable along the lines
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Take away the phase labels and add
POST: @@ tic marks along the lines (the Z axis)
POST: s-lab n
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a z t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-sc z n 500 1000
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 19Ab
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ We will make a new calculation to overlay these monovariant lines
POST: @@ with isothermal calculations
POST: make tcex19a y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY_3: read tcex19a1
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-a-v 3
   ... the command in full is SET_AXIS_VARIABLE
Condition /T/:  none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        16220  grid points in           0  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex19a2 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1300, P=1.01325E5, N=1, X(SI)=0.25, X(AL)=0.2
 DEGREES OF FREEDOM 0
POLY_3: s-c x(al)
   ... the command in full is SET_CONDITION
Value /.2/:  .10
POLY_3: @@ One must use ADD to have several start points at different temperatures.
POLY_3: @@ But do not use default direction as that will create a lot of start points.
POLY_3: @@ Increasing the Si content will most certainly make a solid phase stable.
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: @@ One may have initial equilibria for several different
```

```
POLY_3: @@ conditions at the same time. Just the axis variables have
POLY_3: @@ to be the same
POLY_3: @@ To make nice isothermal curves is not easy, one has to try
POLY_3: @@ with several start points to find all curve sections.
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /1300/:  1200
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        16220  grid points in           0  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /1200/:  1100
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        16220  grid points in           0  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: @@ This line exists only in Al rich corner
POLY_3: s-c x(al)=.5 x(si)=.1
   ... the command in full is SET_CONDITION
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /1100/:  1000
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        16220  grid points in           0  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: @@ A start point in the low melting Al corner too
POLY_3: s-c x(al)=.9 x(si)=.01 t=900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        16220  grid points in           0  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: adva
```

```
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liq
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard

 Phase region boundary   1 at:   5.000E-02  6.891E-01
     LIQUID
  ** DIAMOND_A4
 Calculated           12  equilibria

 Phase region boundary   2 at:   5.000E-02  6.891E-01
     LIQUID
  ** DIAMOND_A4
 Calculated           52  equilibria

 Phase region boundary   3 at:   1.004E-01  3.055E-02
     LIQUID
  ** FCC_A1
 Calculated           21  equilibria

 Phase region boundary   4 at:   1.004E-01  3.055E-02
     LIQUID
  ** FCC_A1
 Calculated.            5  equilibria

       :
       :
       :

 Phase region boundary  36 at:   5.506E-01  5.000E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated.           10  equilibria

 Phase region boundary  37 at:   4.954E-01  4.888E-02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4

 Phase region boundary  38 at:   2.690E-01  5.489E-01
```

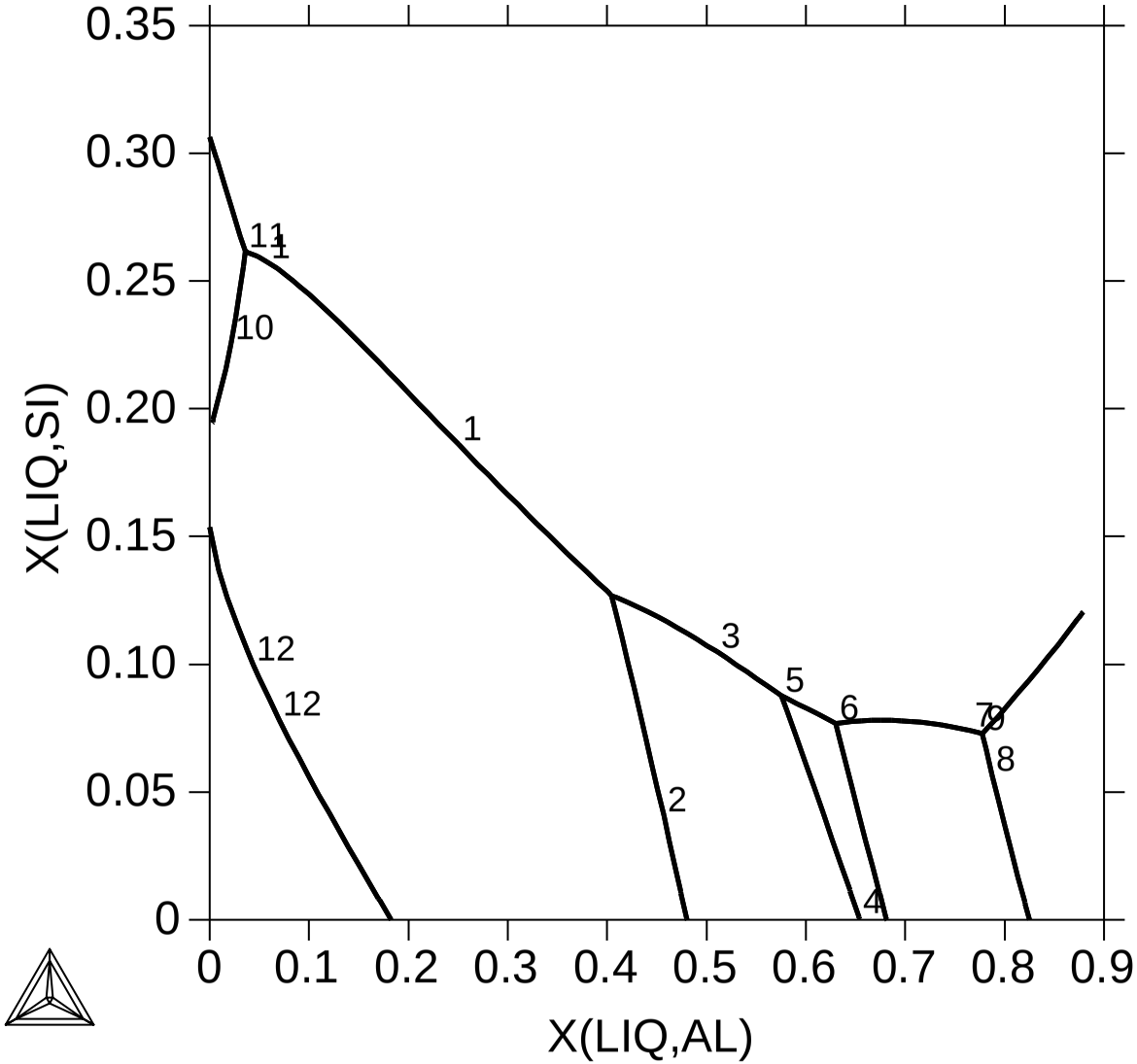
```
    LIQUID
  ** DIAMOND_A4
 Calculated           35  equilibria

 Phase region boundary  39 at:   4.954E-01  4.888E-02
    LIQUID
  ** ALCU_EPSILON
 Calculated           22  equilibria
 *** BUFFER SAVED ON FILE: tcex19a2.POLY3
 CPU time for mapping          17  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

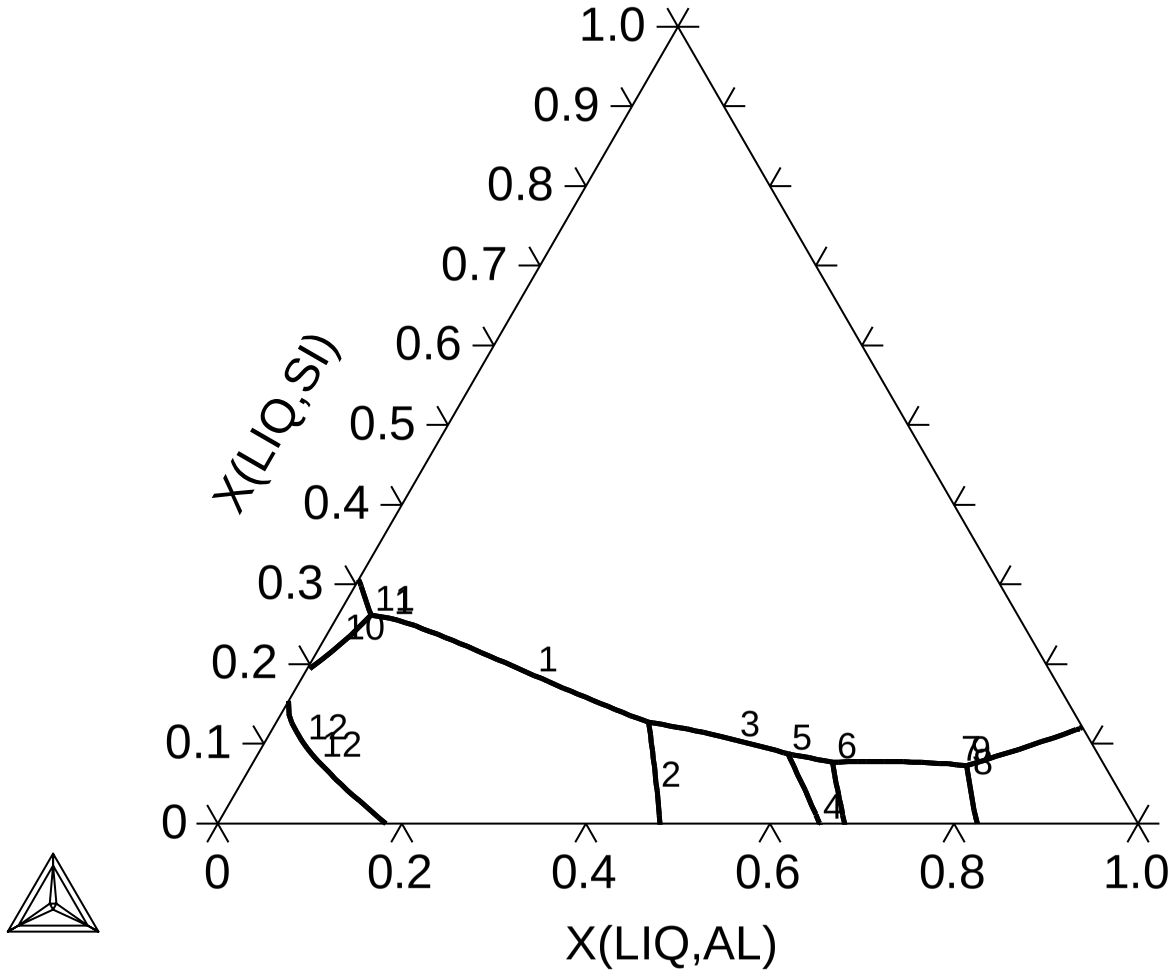
POST: s-d-a x x(liq,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liq,si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-p-f ##1,,,,,,
POST:
POST:
POST: set-title example 19Ac
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: a-e-d y tcex19a
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  1
POST: set-title example 19Ad
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: add .1 .4 n 1300 K
   ... the command in full is ADD_LABEL_TEXT
Text size: /.3999999762/:
POST:
POST: add .1 .3 n 1200 K
   ... the command in full is ADD_LABEL_TEXT
Text size: /.3999999762/:
POST:
POST: set-title example 19Ae
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
 CPU time          21  seconds
```

THERMO-CALC (2009.04.30:12.28) :example 19Aa
DATABASE:USER
P=1.01325E5, N=1.;



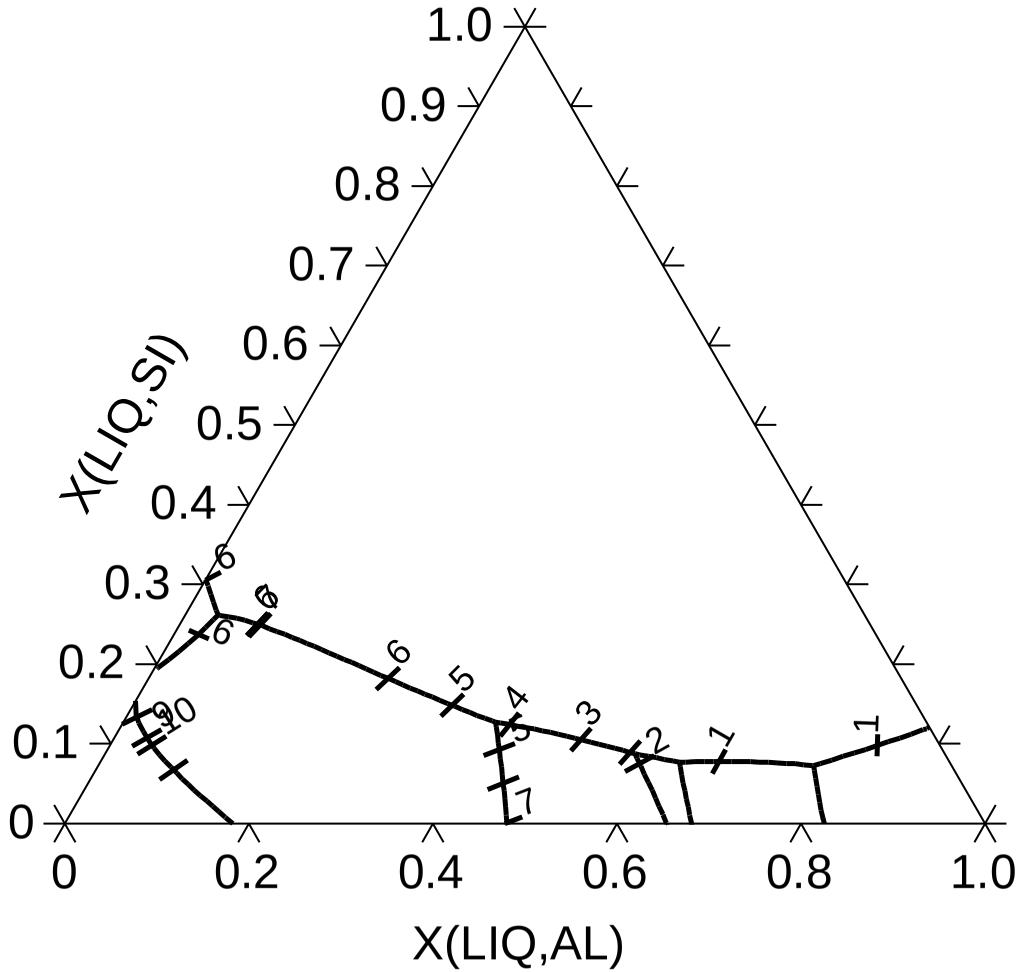
1:*BCC_B2 LIQUID F0 DIAMOND_A4
2:*ALCU_EPSILON LIQUID F0 BCC_B2
3:*ALCU_EPSILON LIQUID F0 DIAMOND_A4
4:*ALCU_EPSILON LIQUID F0 ALCU_ETA
5:*ALCU_ETA LIQUID F0 DIAMOND_A4
6:*ALCU_ETA LIQUID F0 ALCU_THETA
7:*ALCU_THETA LIQUID F0 DIAMOND_A4
8:*ALCU_THETA LIQUID F0 FCC_A1
9:*DIAMOND_A4 LIQUID F0 FCC_A1
10:*BCC_B2 LIQUID F0 CU19SI6_ETA
11:*CU19SI6_ETA LIQUID F0 DIAMOND_A4
12:*BCC_B2 LIQUID F0 FCC_A1

THERMO-CALC (2009.04.30:12.28) :example 19Aa
DATABASE:USER
P=1.01325E5, N=1.;

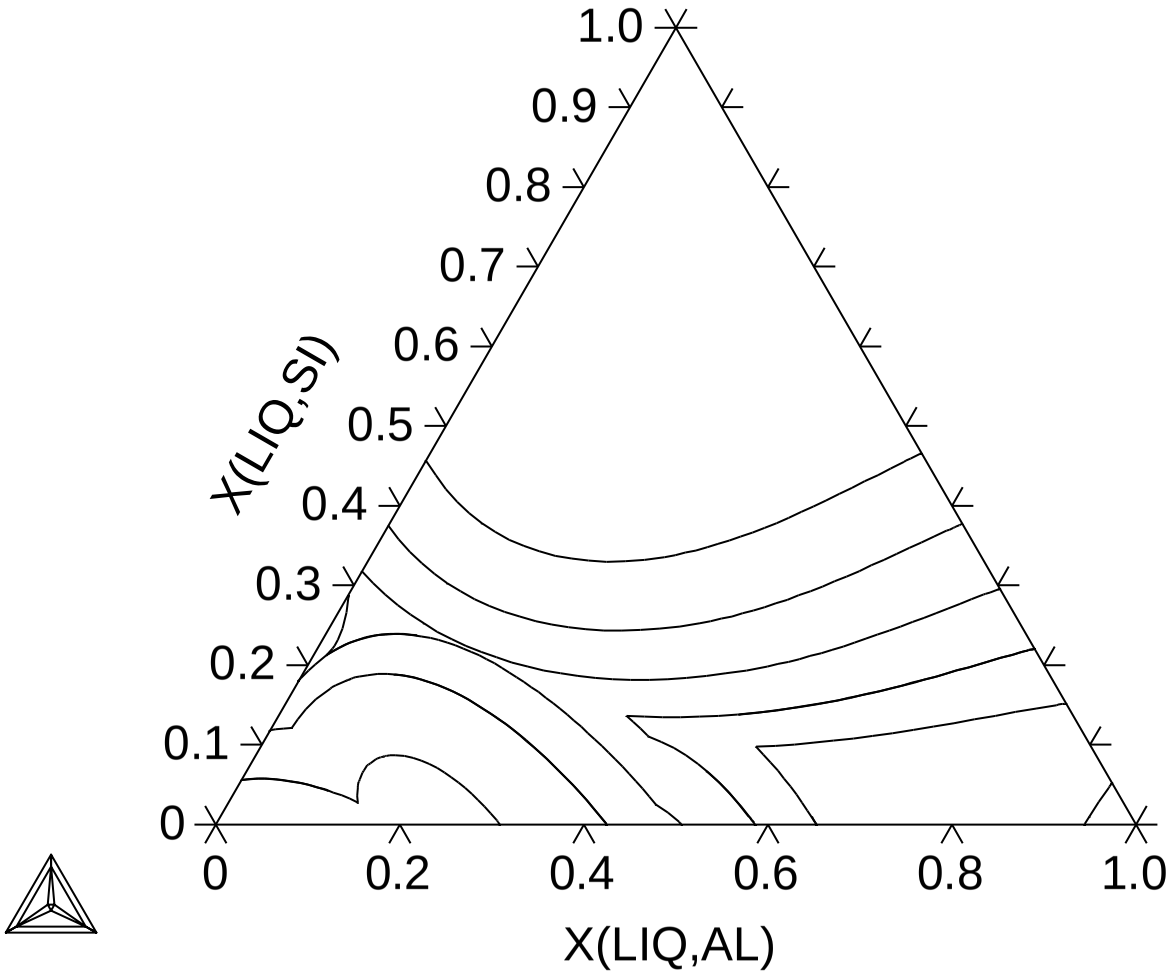


1:*BCC_B2 LIQUID F0 DIAMOND_A4
2:*ALCU_EPSILON LIQUID F0 BCC_B2
3:*ALCU_EPSILON LIQUID F0 DIAMOND_A4
4:*ALCU_EPSILON LIQUID F0 ALCU_ETA
5:*ALCU_ETA LIQUID F0 DIAMOND_A4
6:*ALCU_ETA LIQUID F0 ALCU_THETA
7:*ALCU_THETA LIQUID F0 DIAMOND_A4
8:*ALCU_THETA LIQUID F0 FCC_A1
9:*DIAMOND_A4 LIQUID F0 FCC_A1
10:*BCC_B2 LIQUID F0 CU19SI6_ETA
11:*CU19SI6_ETA LIQUID F0 DIAMOND_A4
12:*BCC_B2 LIQUID F0 FCC_A1

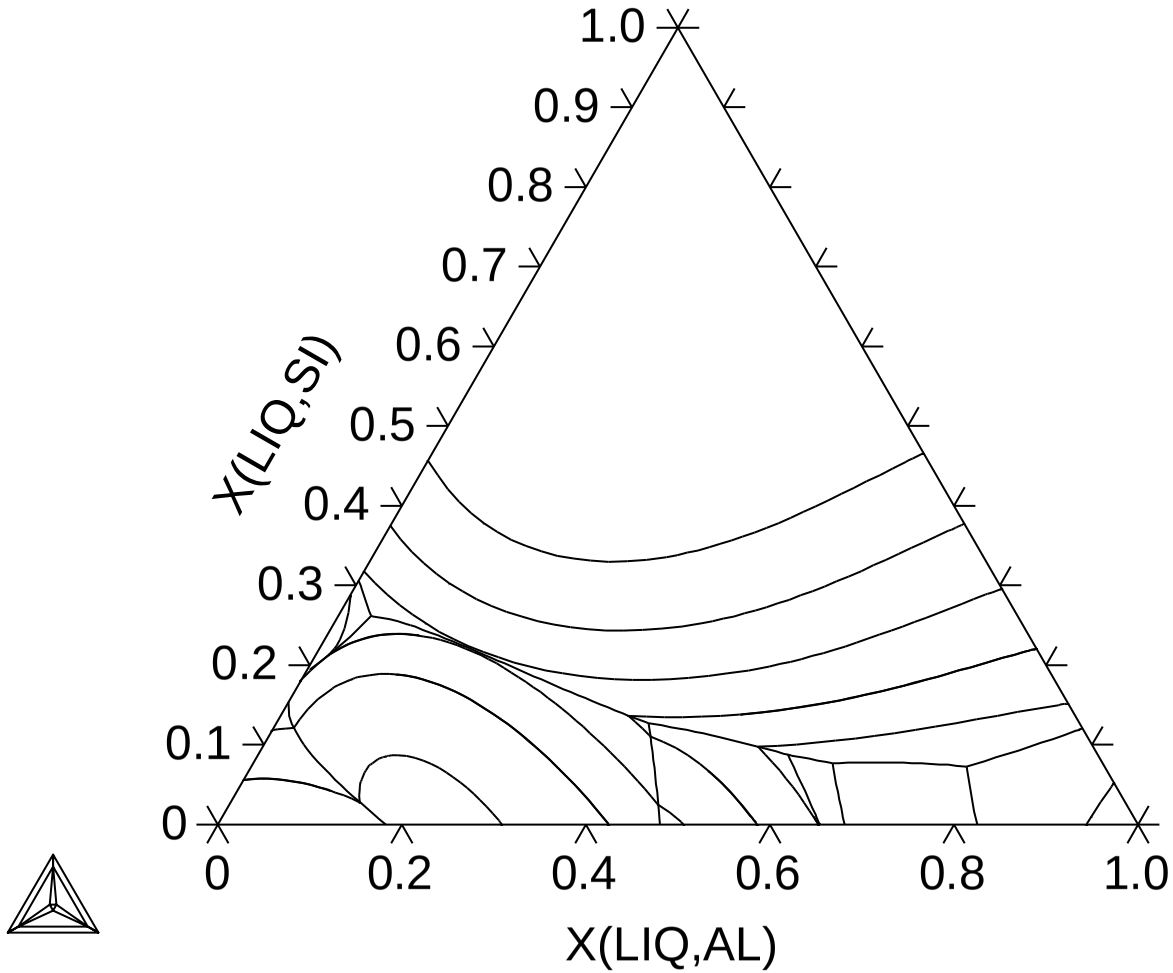
THERMO-CALC (2009.04.30:12.28) :example 19Ab
DATABASE:USER
Z-AXIS = 500.0 + 50.00 * Z



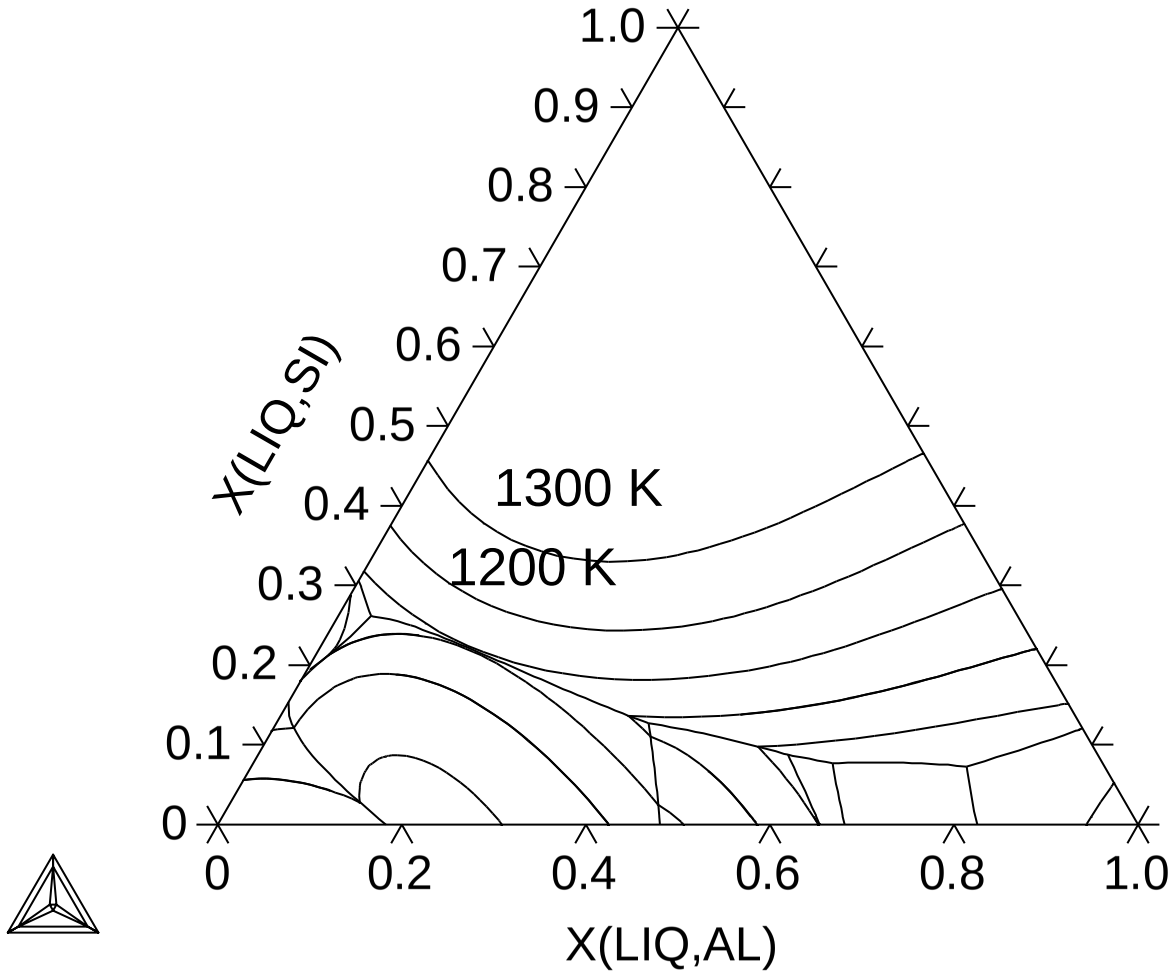
THERMO-CALC (2009.04.30:12.28) :example 19Ac
DATABASE:USER
T=1300, P=1.01325E5, N=1;



THERMO-CALC (2009.04.30:12.28) :example 19Ad
DATABASE:USER
T=1300, P=1.01325E5, N=1;



THERMO-CALC (2009.04.30:12.28) :example 19Ae
DATABASE:USER
T=1300, P=1.01325E5, N=1;



19

Mapping
of univariant equilibria
with the liquid in Al-Cu-Si

Part B. Using TERNARY module

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS: @@    Part B: using TERNARY module
SYS: @@ Using TERNARY module, one can easily obtain the information on
SYS: @@ invariant reactions, such as temperature and compositions.
SYS: @@
SYS: set-log ex19b,,
SYS: go ter
   ... the command in full is GOTO_MODULE

 Quick ternary phase diagram calculation module

 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
Database: /PTERN/:  user
FILENAME: tcex19_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
First element: al cu si
Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/:  L
Min temperature, C /25/:  25
Max temperature, C /2500/:  2500
Temperature interval /100/:  100
Global minimization on: /N/:  N
 VA                      /-  DEFINED
 REINITIATING GES5 .....
 AL                      CU                      SI
   DEFINED
 *** GAS INPUT IGNORED

 ************************************************************
 * WARNING: This database has no list of assessed systems *
 *             The diagram may be wrong.                    *
 ************************************************************

Quit? /Y/:  N
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 Reference REF1       missing
 Reference REF1       missing
 Reference REF1       missing
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
 -OK-
 Forcing automatic start values
```

```
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set
 T = 1673.15 K
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   7.327E-03  9.853E-01
     LIQUID
  ** DIAMOND_A4
 *** Buffer saved on file: MONOVAR.POLY3
 Calculated           15  equilibria

 Phase region boundary   2 at:   7.327E-03  9.853E-01
     LIQUID
  ** DIAMOND_A4
 Calculated           15  equilibria
 *** BUFFER SAVED ON FILE: MONOVAR.POLY3
 CPU time for mapping           1  seconds
 T = 1573.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   7.453E-02  8.883E-01
     LIQUID
  ** DIAMOND_A4
 Calculated           23  equilibria

 Phase region boundary   2 at:   7.453E-02  8.883E-01
     LIQUID
  ** DIAMOND_A4
 Calculated           25  equilibria
 *** BUFFER SAVED ON FILE: MONOVAR.POLY3
 CPU time for mapping           1  seconds
 T = 1473.15 K

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

       :
       :
       :

 Phase region boundary  56 at:   3.646E-02  1.803E-02
     LIQUID
```

```
 ** FCC_A1
Calculated           15  equilibria

Phase region boundary  57 at:   3.646E-02  1.803E-02
    LIQUID
 ** FCC_A1
Calculated           33  equilibria

Phase region boundary  58 at:   4.151E-01  5.493E-03
    LIQUID
 ** ALCU_ETA
Calculated            8  equilibria

Phase region boundary  59 at:   4.151E-01  5.493E-03
    LIQUID
 ** ALCU_ETA
Calculated.           6  equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: MONOVAR.POLY3
CPU time for mapping          12  seconds

 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

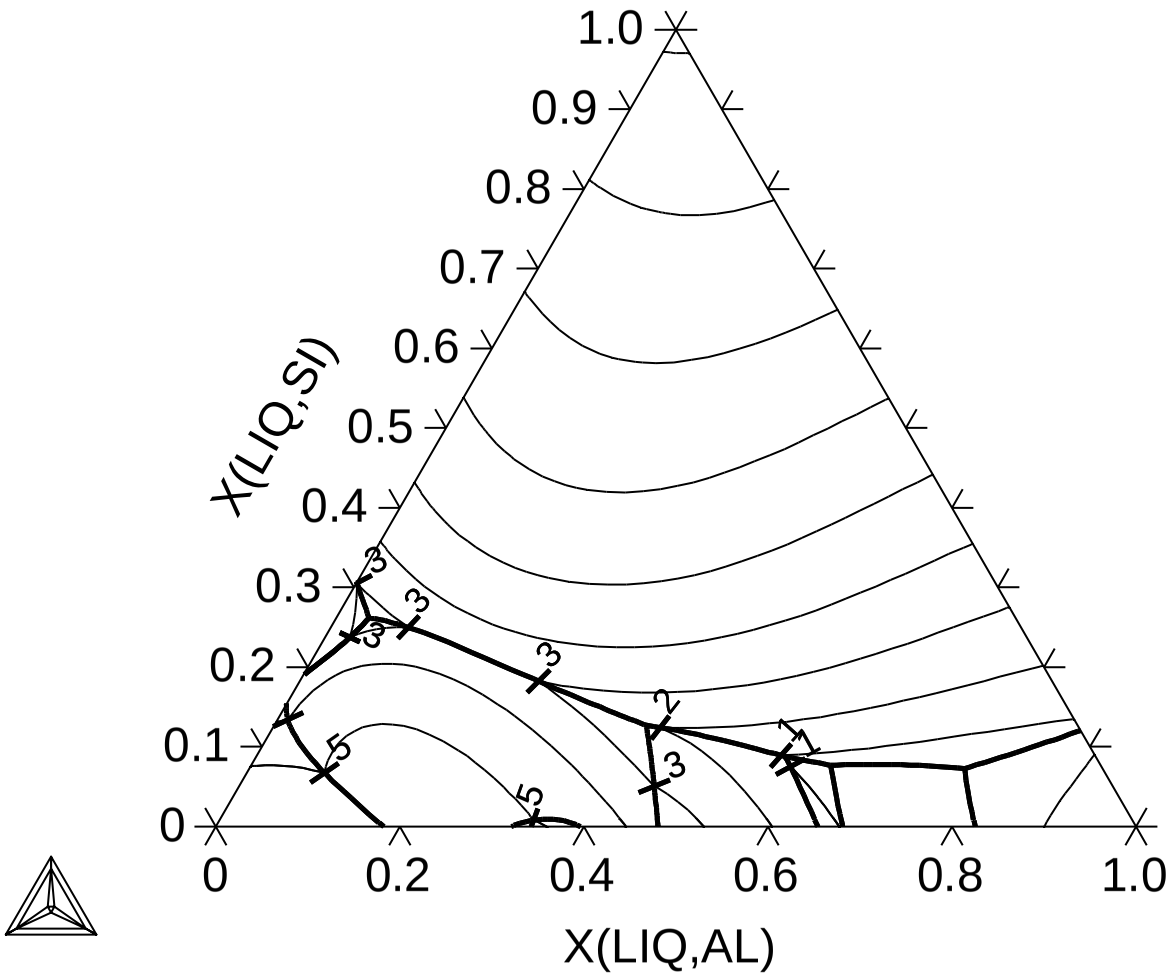
INVARIANT REACTIONS:

E 1:  751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1:  705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2:  594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3:  555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2:  512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1

POST:
POST: s-d-a x x(liq,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,
POST:
POST: set-title example 19B
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:SYS: CPU time           41  seconds
```

THERMO-CALC (2009.04.30:12.30) :example 19B
DATABASE:USER

Z-AXIS = 500.0 + 100.0 * Z



INVARIANT REACTIONS:

E 1 : 751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAM
U 1 : 705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DI
U 2 : 594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA +
U 3 : 555.98 C: LIQUID + ALCU_ETA -> ALCU_THE +
E 2 : 512.07 C: LIQUID -> ALCU_THE + DIAMOND + F

20

Calculation of adiabatic decompression in a geological system

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example showing how to calculate an adiabatic decompression
SYS: @@ using the geochemical database
SYS: @@
SYS: set-log ex20,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw pgeo
   ... the command in full is SWITCH_DATABASE
 Current database: Saxena Pure Minerals Database v1

 O                       VA  DEFINED
 STEAM                   OXYGEN                  HYDROGEN
   REJECTED
 CARBON_MONOXIDE         CARBON_DIOXIDE          METHANE
   REJECTED
TDB_PGEO: d-sys mg si
   ... the command in full is DEFINE_SYSTEM
 MG                      SI  DEFINED
TDB_PGEO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 GAS:G       :O2:
  > Gaseous Mixture with C-H-O species, using ideal gas model
 A_QUARTZ    :SI1O2:
 B_QUARTZ    :SI1O2:
 CRISTOBALITE :SI1O2:
 TRIDYMITE   :SI1O2:
 COESITE     :SI1O2:
 STISHOVITE  :SI1O2:
 PERICLASE   :MG1O1:
 FORSTERITE  :SI1MG2O4:
 BETA_FORSTERITE :SI1MG2O4:
 GAMMA_FORSTERITE :SI1MG2O4:
 ILMENITE_MG :SI1MG1O3:
 MG_PEROVSKITE :SI1MG1O3:
 CLINOENSTATITE :SI1MG1O3:
 ORTHOENSTATITE :SI1MG1O3:
 PROTOENSTATITE :SI1MG1O3:
 CLINOENSTHP :SI1MG1O3:
 GARNET_MG   :SI1MG1O3:
TDB_PGEO: rej ph gas proto
   ... the command in full is REJECT
 GAS:G                   PROTOENSTATITE  REJECTED
TDB_PGEO: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_PGEO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ We define more convenient components
POLY_3: def-com mgo o sio2
```

```
   ... the command in full is DEFINE_COMPONENTS
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:  CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 MGO                     ENTERED   SER
 O                       ENTERED   SER
 SIO2                    ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 TRIDYMITE               ENTERED    0.00000000E+00  0.00000000E+00
 STISHOVITE              ENTERED    0.00000000E+00  0.00000000E+00
 PERICLASE               ENTERED    0.00000000E+00  0.00000000E+00
 ORTHOENSTATITE          ENTERED    0.00000000E+00  0.00000000E+00
 MG_PEROVSKITE           ENTERED    0.00000000E+00  0.00000000E+00
 ILMENITE_MG             ENTERED    0.00000000E+00  0.00000000E+00
 GARNET_MG               ENTERED    0.00000000E+00  0.00000000E+00
 GAMMA_FORSTERITE        ENTERED    0.00000000E+00  0.00000000E+00
 FORSTERITE              ENTERED    0.00000000E+00  0.00000000E+00
 CRISTOBALITE            ENTERED    0.00000000E+00  0.00000000E+00
 COESITE                 ENTERED    0.00000000E+00  0.00000000E+00
 CLINOENSTHP             ENTERED    0.00000000E+00  0.00000000E+00
 CLINOENSTATITE          ENTERED    0.00000000E+00  0.00000000E+00
 B_QUARTZ                ENTERED    0.00000000E+00  0.00000000E+00
 BETA_FORSTERITE         ENTERED    0.00000000E+00  0.00000000E+00
 A_QUARTZ                ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 MG       ENTERED    O        ENTERED    SI1MG1O3 ENTERED    SIO2     ENTERED
 MG1O1    ENTERED    O2       ENTERED    SI1MG2O4 ENTERED    VA       ENTERED
 MGO      ENTERED    SI       ENTERED    SI1O2    ENTERED
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ and specify a composition assumed to be
POLY_3: @@ present in the earth mantle
POLY_3: s-i-a n(mgo)=80
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-i-a n(si1mg1o3)=100
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(MGO)=180, N(SIO2)=100
 DEGREES OF FREEDOM 3
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ There is an error if mgsio3 is used instead of the defined si1mg1o3,
POLY_3: @@ since mgsio3 is not defined as a species.
POLY_3: s-c t=2200,p=2e10
   ... the command in full is SET_CONDITION
POLY_3: save tcex20 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @@ We have no degree of freedom with respect
POLY_3: @@ to oxygen so set its activity to unity (or
POLY_3: @@ any positive number)
POLY_3: s-c ac(o)=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated           16  grid points in            0  s
    31 ITS,  CPU TIME USED   0 SECONDS
POLY_3: save tcex20 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 GARNET_MG               ENTERED    0.00000000E+00  4.00000000E+01
 BETA_FORSTERITE         ENTERED    0.00000000E+00  2.40000000E+02
 GAMMA_FORSTERITE        ENTERED   -5.94672975E-03  0.00000000E+00
 MG_PEROVSKITE           ENTERED   -2.55835159E-02  0.00000000E+00
 ILMENITE_MG             ENTERED   -4.82844546E-02  0.00000000E+00
 PERICLASE               ENTERED   -9.57514325E-02  0.00000000E+00
 CLINOENSTHP             ENTERED   -1.54163155E-01  0.00000000E+00
```

```
 ORTHOENSTATITE          ENTERED   -2.19745018E-01  0.00000000E+00
 CLINOENSTATITE          ENTERED   -2.39436864E-01  0.00000000E+00
 FORSTERITE              ENTERED   -2.41718999E-01  0.00000000E+00
 STISHOVITE              ENTERED   -3.05398375E-01  0.00000000E+00
 COESITE                 ENTERED   -3.77531570E+00  0.00000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN -7.83559188E+00
 A_QUARTZ B_QUARTZ TRIDYMITE CRISTOBALITE
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  X
 Output from POLY-3, equilibrium =     1, label A0  , database: PGEO

 Conditions:
 N(MGO)=180, N(SIO2)=100, T=2200, P=2E10, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature   2200.00 K (  1926.85 C),  Pressure  2.000000E+10
 Number of moles of components  2.80000E+02,  Mass in grams  1.32632E+04
 Total Gibbs energy -1.80863E+08,  Enthalpy -9.91578E+07,  Volume  3.55512E-03

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 MGO                     1.8000E+02  6.4286E-01 7.6674E-14 -5.5240E+05 SER
 O                       0.0000E+00  0.0000E+00 1.0000E+00  0.0000E+00 SER
 SIO2                    1.0000E+02  3.5714E-01 4.6393E-20 -8.1430E+05 SER

 BETA_FORSTERITE             Status ENTERED     Driving force  0.0000E+00
 Moles 2.4000E+02, Mass 1.1255E+04, Volume fraction 8.5320E-01  Mole fractions:
 MGO   6.66667E-01  SIO2  3.33333E-01  O     0.00000E+00

 GARNET_MG                   Status ENTERED     Driving force  0.0000E+00
 Moles 4.0000E+01, Mass 2.0078E+03, Volume fraction 1.4680E-01  Mole fractions:
 MGO   5.00000E-01  SIO2  5.00000E-01  O     0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: ent fun dens=1e-3*bm/vm;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh dens
   ... the command in full is SHOW_VALUE
 DENS=3730.7358
POLY_3: @@ We have now found the equilibrium at this
POLY_3: @@ pressure. Now assume this system is decompressed
POLY_3: @@ adiabatically. What will the new temperature become?
POLY_3: s-c h
   ... the command in full is SET_CONDITION
Value /-99157833.21/:
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /2200/:  none
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(MGO)=180, N(SIO2)=100, P=2E10, AC(O)=1, H=-9.91578E7
 DEGREES OF FREEDOM 0
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Now t is independent, calculate the equilibrium and get t
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated           16  grid points in            0  s
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=2200.
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ No big surprise! the same temperature. Now change pressure
POLY_3: s-c p
   ... the command in full is SET_CONDITION
Value /2E+10/:  150e8
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated           16  grid points in            0  s
    17 ITS,  CPU TIME USED   0 SECONDS
```

```
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=2977.6276
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ We will also have a new density and another set of
POLY_3: @@ stable phases.
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VXCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: PGEO

 Conditions:
 N(MGO)=180, N(SIO2)=100, P=1.5E10, AC(O)=1, H=-9.91578E7
 DEGREES OF FREEDOM 0

 Temperature   2977.63 K (  2704.48 C),  Pressure  1.500000E+10
 Number of moles of components  2.80000E+02,  Mass in grams  1.32632E+04
 Total Gibbs energy -2.30661E+08,  Enthalpy -9.91578E+07,  Volume  3.59115E-03

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 MGO                     1.8000E+02  6.4286E-01 4.6875E-13 -7.0283E+05 SER
 O                       0.0000E+00  0.0000E+00 1.0000E+00  0.0000E+00 SER
 SIO2                    1.0000E+02  3.5714E-01 5.3688E-19 -1.0415E+06 SER

 GARNET_MG                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.0000E+02, Mass 1.0039E+04, Volume fraction 7.4847E-01  Mole fractions:
 MGO   5.00000E-01  SIO2  5.00000E-01  O     0.00000E+00

 PERICLASE                   Status ENTERED     Driving force  0.0000E+00
 Moles 8.0000E+01, Mass 3.2244E+03, Volume fraction 2.5153E-01  Mole fractions:
 MGO   1.00000E+00  SIO2  0.00000E+00  O     0.00000E+00
POLY_3: sh dens
   ... the command in full is SHOW_VALUE
 DENS=3693.3029
POLY_3: sh v
   ... the command in full is SHOW_VALUE
 V=3.5911547E-3
POLY_3: sh vm
   ... the command in full is SHOW_VALUE
 VM=1.2825553E-5
POLY_3:
POLY_3:@?
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3: CPU time            1  seconds
```

21

Calculation
with a user defined database

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Show the use of your own database
SYS: @@ Calculate a ternary isotherm in Fe-Cr-Ni with a user database
SYS: @@
SYS: set-log ex21,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw user tcex21
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA  DEFINED
TDB_USER: def-sys *
   ... the command in full is DEFINE_SYSTEM
 /-                      VA                      CR
 FE                      NI  DEFINED
TDB_USER: li-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 LIQUID:L    :CR FE NI:
 BCC_A2      :CR FE NI:VA:
 FCC_A1      :CR FE NI:VA:
 HCP_A3      :CR FE NI:VA:
 SIGMA       :FE NI:CR:CR FE NI:
TDB_USER: @?<Hit_return_to_continue>
TDB_USER: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A.T. Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4, p 317-425; '
  'J.O. Andersson, B. Sundman, Calphad 11(1987)1 p 83-92 TRITA-MAC 270
      (1986); Cr-Fe'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'Byeong-Joo Lee, Calphad 16(1992)2, p 121-149; carbides'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Fe-Ni'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Cr-Ni'
  'A.F. Guillermet, Z. Metallkde. 79(1988)8 p 524-536, TRITA-MAC 362 (1988);
      C-Co-Ni, C-Co-Fe-Ni'
  'K. Frisk, Metall. Trans. 21A (1990)9 p 2477-2488, Cr-Fe-N'
  'Unassessed parameter, linear combination of unary data.'
  'P. Gustafson, Calphad 12(1987)3 p 277-292, Cr-Ni-W '
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ With 3 components we must set 5 conditions
POLY_3: s-c t=1073 p=1e5 n=1 x(cr)=.2 x(ni)=.2
   ... the command in full is SET_CONDITION
POLY_3: l-c
```

```
   ... the command in full is LIST_CONDITIONS
 T=1073, P=1E5, N=1, X(CR)=0.2, X(NI)=0.2
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         9315  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1073, P=1E5, N=1, X(CR)=0.2, X(NI)=0.2
 DEGREES OF FREEDOM 0

 Temperature   1073.00 K (   799.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.56454E+01
 Total Gibbs energy -5.39559E+04,  Enthalpy  3.01555E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      2.0000E-01  1.8688E-01 5.8626E-03 -4.5849E+04 SER
 FE                      6.0000E-01  6.0217E-01 3.1002E-03 -5.1533E+04 SER
 NI                      2.0000E-01  2.1094E-01 4.2164E-04 -6.9332E+04 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.5645E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  6.02174E-01  NI  2.10943E-01  CR  1.86883E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Define axis
POLY_3: s-a-v 1 x(cr) 0 1,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(ni) 0 1,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex21 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 ERROR         1611  when calculating equilibrium
 ERROR         1611  when calculating equilibrium
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
```

```
 Generating start point  16
 Generating start point  17
 Generating start point  18

 Phase region boundary   1 at:   3.521E-02  1.510E-02
     BCC_A2
  ** FCC_A1
 *** Buffer saved on file: tcex21.POLY3
 Calculated.           20  equilibria

 Phase region boundary   2 at:   2.615E-01  6.190E-02
     BCC_A2
  ** FCC_A1
  ** SIGMA

 Phase region boundary   3 at:   3.723E-01  3.566E-02
     BCC_A2
  ** SIGMA
 Calculated           21  equilibria

 Phase region boundary   4 at:   3.168E-01  6.107E-02
     FCC_A1
  ** SIGMA
 Calculated.           20  equilibria

       :
       :
       :

 Phase region boundary  22 at:   6.363E-01  2.710E-01
  ** BCC_A2
     FCC_A1
 Calculated.           16  equilibria
 Terminating at known equilibrium

 Phase region boundary  23 at:   6.363E-01  2.710E-01
  ** BCC_A2
     FCC_A1
 Calculated           26  equilibria

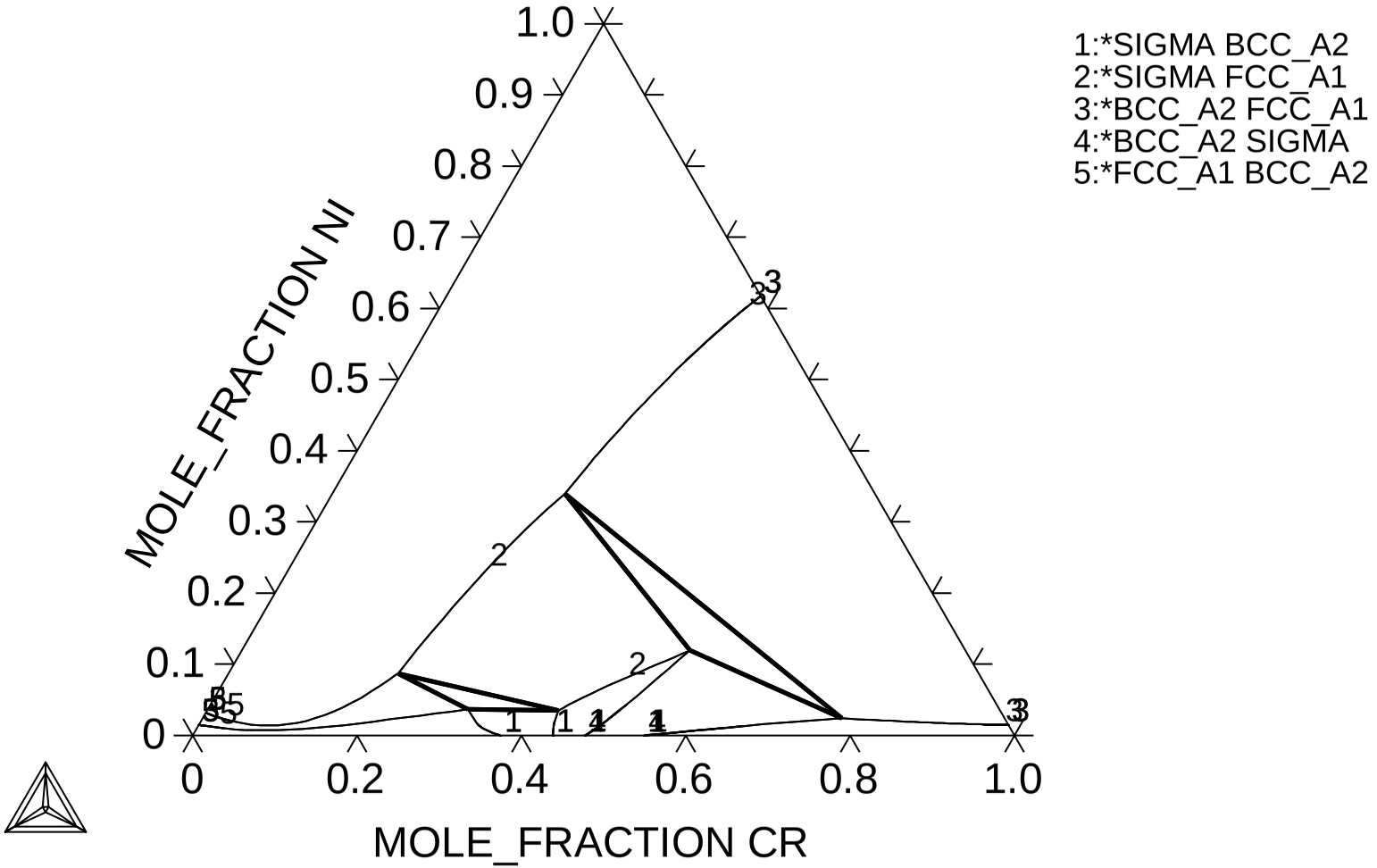
 Phase region boundary  24 at:   6.789E-01  3.114E-01
  ** BCC_A2
     FCC_A1
 Calculated.           22  equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   6.789E-01  3.114E-01
  ** BCC_A2
     FCC_A1
 Calculated           16  equilibria
 *** BUFFER SAVED ON FILE: tcex21.POLY3
 CPU time for mapping           5  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST:
POST: set-title example 21a
POST: se-d-ty y,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-l b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time            6  seconds
```

THERMO-CALC (2009.04.22:16.19) :example 21a
DATABASE:USER
T=1073, P=1E5, N=1;



22

Calculation of heat balance

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of a heat balance. In this case C3H8 is burned in
SYS: @@ oxygen and the adiabatic flame temperature is calculated.
SYS: @@
SYS: set-log ex22,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw ssub4
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v4

 VA  DEFINED
TDB_SSUB4: def-sys c o h
   ... the command in full is DEFINE_SYSTEM
 C                       O                       H
   DEFINED
TDB_SSUB4: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
   C1H1<G> T.C.R.A.S. Class: 2
   C1H1O1<G> T.C.R.A.S. Class: 4
      FORMYL <GAS>
   C1H1O2<G> T.C.R.A.S. Class: 6
   C1H2<G> T.C.R.A.S. Class: 5
      METHYLENE <GAS>
                    :
                    :
                    :
   C1<DIAMOND> S.G.T.E. **
      <DIAMOND>
      Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
      from 1994 database (ex THERMODATA 01/93)
   H2O1 T.C.R.A.S. Class: 4
      WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002
   H2O2 THERMODATA 01/93
      HYDROGEN PEROXIDE
      28/01/93
 -OK-
TDB_SSUB4: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       ENTERED   SER
```

```
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 H2O2_L                  ENTERED    0.00000000E+00  0.00000000E+00
 H2O1_L                  ENTERED    0.00000000E+00  0.00000000E+00
 DIAMOND                 ENTERED    0.00000000E+00  0.00000000E+00
 C_S                     ENTERED    0.00000000E+00  0.00000000E+00
 C_L                     ENTERED    0.00000000E+00  0.00000000E+00
 C6H6_L                  ENTERED    0.00000000E+00  0.00000000E+00
 C60_S                   ENTERED    0.00000000E+00  0.00000000E+00
 C2H6O2_L                ENTERED    0.00000000E+00  0.00000000E+00
 C2H6O1_L                ENTERED    0.00000000E+00  0.00000000E+00
 C2H4O2_L                ENTERED    0.00000000E+00  0.00000000E+00
 C1H4O1_L                ENTERED    0.00000000E+00  0.00000000E+00
 C1H2O2_L                ENTERED    0.00000000E+00  0.00000000E+00
 GAS                     ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 C                    ENTERED    C3H4_2               ENTERED
 C1H1                 ENTERED    C3H6                 ENTERED
 C1H1O1               ENTERED    C3H6O1               ENTERED
 C1H1O2               ENTERED    C3H6_2               ENTERED
 C1H2                 ENTERED    C3H8                 ENTERED
 C1H2O1               ENTERED    C3O2                 ENTERED
 C1H2O2               ENTERED    C4                   ENTERED
 C1H2O2_CIS           ENTERED    C4H1                 ENTERED
 C1H2O2_DIOXIRANE     ENTERED    C4H10_1              ENTERED
 C1H2O2_TRANS         ENTERED    C4H10_2              ENTERED
 C1H3                 ENTERED    C4H2                 ENTERED
 C1H3O1_CH2OH         ENTERED    C4H4                 ENTERED
 C1H3O1_CH3O          ENTERED    C4H4_1_3             ENTERED
 C1H4                 ENTERED    C4H6_1               ENTERED
 C1H4O1               ENTERED    C4H6_2               ENTERED
 C1O1                 ENTERED    C4H6_3               ENTERED
 C1O2                 ENTERED    C4H6_4               ENTERED
 C2                   ENTERED    C4H6_5               ENTERED
 C2H1                 ENTERED    C4H8                 ENTERED
 C2H2                 ENTERED    C4H8_1               ENTERED
 C2H2O1               ENTERED    C4H8_2               ENTERED
 C2H3                 ENTERED    C4H8_3               ENTERED
 C2H4                 ENTERED    C4H8_4               ENTERED
 C2H4O1_ACETALDEHYDE  ENTERED    C4H8_5               ENTERED
 C2H4O1_OXIRANE       ENTERED    C5                   ENTERED
 C2H4O2               ENTERED    C60                  ENTERED
 C2H4O2_ACETICACID    ENTERED    C6H6                 ENTERED
 C2H4O2_DIOXETANE     ENTERED    C6H6O1               ENTERED
 C2H4O3_123TRIOXOLANE ENTERED    H                    ENTERED
 C2H4O3_124TRIOXOLANE ENTERED    H1O1                 ENTERED
 C2H5                 ENTERED    H1O2                 ENTERED
 C2H6                 ENTERED    H2                   ENTERED
 C2H6O1               ENTERED    H2O1                 ENTERED
 C2H6O2               ENTERED    H2O2                 ENTERED
 C2O1                 ENTERED    O                    ENTERED
 C3                   ENTERED    O2                   ENTERED
 C3H1                 ENTERED    O3                   ENTERED
 C3H4_1               ENTERED    VA                   ENTERED
POLY_3: @@ We need to know the heat content of C3H8<G> at room temperature.
POLY_3: @@ This is a simple number to look up in a table but actually quite
POLY_3: @@ tricky to calculate as pure C3H8 at room temperature does not
POLY_3: @@ represent an equilibrium state. However, one can obtain it by
POLY_3: @@ the following procedure.
POLY_3: s-c t=298.15,p=1e5,n(o)=1e-10
   ... the command in full is SET_CONDITION
POLY_3: s-i-a n(c3h8)=1
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: c-s p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-s p gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
```

```
 Calculated           73  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: @@ The equilibrium state at room temperature is listed
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB4

 Conditions:
 T=298.15, P=1E5, N(O)=1E-10, N(C)=3, N(H)=8
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.10000E+01,  Mass in grams  4.40962E+01
 Total Gibbs energy -2.20108E+05,  Enthalpy -1.06064E+05,  Volume  4.99502E-02

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.0000E+00  8.1715E-01 1.1356E+07  4.0271E+04 SER
 H                       8.0000E+00  1.8285E-01 3.4211E-08 -4.2615E+04 SER
 O                       1.0000E-10  3.6282E-11 1.2651E-49 -2.7911E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 1.1000E+01, Mass 4.4096E+01, Volume fraction 1.0000E+00  Mass fractions:
 C  8.17145E-01  H  1.82855E-01  O  3.62820E-11
 Constitution:
 C1H4          9.90348E-01  C2H6O1        1.83029E-24  C2H4O1_OXIRA 1.00000E-30
 C60           8.16678E-03  C1H4O1        1.08754E-24  C4H6_5       1.00000E-30
 C6H6          1.38456E-03  C1H2O1        4.96084E-27  C5           1.00000E-30
 C2H6          1.00313E-04  C1H2O2_CIS    4.88436E-27  C2H3         1.00000E-30
 C3H8          5.44582E-07  C4H6_4        3.94602E-28  C2H2O1       1.00000E-30
 C4H10_2       3.84975E-08  C3H4_2        6.04110E-29  C2H2         1.00000E-30
 H2            7.83769E-09  C2H5          1.32230E-29  C2H1         1.00000E-30
 C4H10_1       6.16323E-09  C1H2O2_TRANS  6.61825E-30  C2           1.00000E-30
 C1O2          2.32090E-11  C3H4_1        2.45341E-30  H            1.00000E-30
 H2O1          2.50979E-12  C4H6_1        2.07866E-30  H1O1         1.00000E-30
 C1O1          7.01016E-13  C             1.00000E-30  H1O2         1.00000E-30
 C4H8_5        6.25907E-14  C3O2          1.00000E-30  H2O2         1.00000E-30
 C3H6_2        5.52670E-14  C4            1.00000E-30  C1H3O1_CH3O  1.00000E-30
 C3H6          5.28022E-14  C4H1          1.00000E-30  C1H3O1_CH2OH 1.00000E-30
 C2H4          3.33175E-14  C3H1          1.00000E-30  C1H3         1.00000E-30
 C4H8_3        8.77188E-15  C3            1.00000E-30  O            1.00000E-30
 C4H8_2        2.73753E-15  C2O1          1.00000E-30  C1H2O2_DIOXI 1.00000E-30
 C4H8_1        3.05059E-16  C2H6O2        1.00000E-30  O2           1.00000E-30
 C6H6O1        1.02341E-18  C4H2          1.00000E-30  O3           1.00000E-30
 C3H6O1        9.99430E-20  C4H4          1.00000E-30  C1H2         1.00000E-30
 C4H6_2        4.91032E-22  C4H4_1_3      1.00000E-30  C1H1O2       1.00000E-30
 C2H4O1_ACETA 1.25014E-22  C2H4O3_124TR 1.00000E-30  C1H1O1       1.00000E-30
 C4H8          4.93171E-23  C2H4O3_123TR 1.00000E-30  C1H1         1.00000E-30
 C4H8_4        2.16142E-23  C2H4O2_DIOXE 1.00000E-30
 C2H4O2_ACETI 9.64309E-24  C4H6_3        1.00000E-30
POLY_3: @@ The enthalpy for the system is
POLY_3: sh h
   ... the command in full is SHOW_VALUE
 H=-106064.27
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ But we want a gas with just C3H8. Use the set-all-startvalues command.
POLY_3: s-a-s
   ... the command in full is SET_ALL_START_VALUES
Automatic start values for phase constituents? /N/:  n
Should GAS be stable? /Y/:  1
Major constituent(s):  C3H8
POLY_3: sh h
   ... the command in full is SHOW_VALUE
 H=-99422.043
POLY_3: @@ The difference in H for the two calculations is actually not very large.
POLY_3: @@ The value is approximate but rather good as the enthalpy is calculated
POLY_3: @@ for the following gas constitution
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB4

 Conditions:
 T=298.15, P=1E5, N(O)=1E-10, N(C)=3, N(H)=8
 DEGREES OF FREEDOM 0
```

```
 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.07453E+01,  Mass in grams  4.32990E+01
 Total Gibbs energy -1.78567E+05,  Enthalpy -9.94220E+04,  Volume  2.43003E-02

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.9417E+00  8.1603E-01 1.1356E+07  4.0271E+04 SER
 H                       7.7969E+00  1.8149E-01 3.4211E-08 -4.2615E+04 SER
 O                       6.7123E-03  2.4802E-03 1.2651E-49 -2.7911E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 1.0745E+01, Mass 4.3299E+01, Volume fraction 1.0000E+00  Mass fractions:
 C  8.16027E-01  H  1.81493E-01  O  2.48021E-03
 Constitution:
 C3H8         9.70396E-01  C4H4_1_3     1.36986E-04  C2H4O1_OXIRA 1.36986E-04
 C            1.36986E-04  C4H4         1.36986E-04  C2H4O1_ACETA 1.36986E-04
 O2           1.36986E-04  C4H2         1.36986E-04  C2H4         1.36986E-04
 O            1.36986E-04  C4H10_2      1.36986E-04  C2H3         1.36986E-04
 H2O2         1.36986E-04  C4H10_1      1.36986E-04  C2H2O1       1.36986E-04
 H2O1         1.36986E-04  C4H1         1.36986E-04  C2H2         1.36986E-04
 H2           1.36986E-04  C4           1.36986E-04  C2H1         1.36986E-04
 H1O2         1.36986E-04  C3O2         1.36986E-04  C2           1.36986E-04
 H1O1         1.36986E-04  O3           1.36986E-04  C1O2         1.36986E-04
 H            1.36986E-04  C3H6_2       1.36986E-04  C1O1         1.36986E-04
 C6H6O1       1.36986E-04  C3H6O1       1.36986E-04  C1H4O1       1.36986E-04
 C6H6         1.36986E-04  C3H6         1.36986E-04  C1H4         1.36986E-04
 C60          1.36986E-04  C3H4_2       1.36986E-04  C1H3O1_CH3O  1.36986E-04
 C5           1.36986E-04  C3H4_1       1.36986E-04  C1H3O1_CH2OH 1.36986E-04
 C4H8_5       1.36986E-04  C3H1         1.36986E-04  C1H3         1.36986E-04
 C4H8_4       1.36986E-04  C3           1.36986E-04  C1H2O2_TRANS 1.36986E-04
 C4H8_3       1.36986E-04  C2O1         1.36986E-04  C1H2O2_DIOXI 1.36986E-04
 C4H8_2       1.36986E-04  C2H6O2       1.36986E-04  C1H2O2_CIS   1.36986E-04
 C4H8_1       1.36986E-04  C2H6O1       1.36986E-04  C1H2O1       1.36986E-04
 C4H8         1.36986E-04  C2H6         1.36986E-04  C1H2         1.36986E-04
 C4H6_5       1.36986E-04  C2H5         1.36986E-04  C1H1O2       1.36986E-04
 C4H6_4       1.36986E-04  C2H4O3_124TR 1.36986E-04  C1H1O1       1.36986E-04
 C4H6_3       1.36986E-04  C2H4O3_123TR 1.36986E-04  C1H1         1.36986E-04
 C4H6_2       1.36986E-04  C2H4O2_DIOXE 1.36986E-04
 C4H6_1       1.36986E-04  C2H4O2_ACETI 1.36986E-04
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ We now have the initial amount of heat. Assuming an excess
POLY_3: @@ of oxygen we can calulate the temperature where the
POLY_3: @@ heat content whould be the same
POLY_3: sh h
   ... the command in full is SHOW_VALUE
 H=-99422.043
POLY_3: @@ H is just 11 times HM as there are 11 atoms in C3H8, save that value
POLY_3: @@ in a variable
POLY_3: enter var h298=h;
   ... the command in full is ENTER_SYMBOL
POLY_3: sh h298
   ... the command in full is SHOW_VALUE
 H298=-99422.043
POLY_3: @@ If all carbon and hydrogen react with oxygen we need 7 oxygen atoms
POLY_3: @@ to form 3 moles C1O and 4 moles of H2O, add some oxygen in excess
POLY_3: s-c n(o)=9
   ... the command in full is SET_CONDITION
POLY_3: @@ Set the heat content as condition and remove the condition on t
POLY_3: s-c h=h298
   ... the command in full is SET_CONDITION
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /298.15/:  none
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, N(O)=9, N(C)=3, N(H)=8, H=H298
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated           73  grid points in           0  s
   153 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
```

```
  ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB4

 Conditions:
 P=1E5, N(O)=9, N(C)=3, N(H)=8, H=H298
 DEGREES OF FREEDOM 0

 Temperature   3103.40 K (  2830.25 C),  Pressure  1.000000E+05
 Number of moles of components  2.00000E+01,  Mass in grams  1.88087E+02
 Total Gibbs energy -7.70697E+06,  Enthalpy -9.94220E+04,  Volume  2.20474E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.0000E+00  1.9158E-01 9.3954E-09 -4.7692E+05 SER
 H                       8.0000E+00  4.2869E-02 7.7619E-06 -3.0361E+05 SER
 O                       9.0000E+00  7.6555E-01 6.3831E-08 -4.2748E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 2.0000E+01, Mass 1.8809E+02, Volume fraction 1.0000E+00  Mass fractions:
 O  7.65554E-01  C  1.91576E-01  H  4.28695E-02
 Constitution:
 H2O1          3.17921E-01  C2H2          1.14584E-15  C3H6O1        1.00000E-30
 C1O1          2.27786E-01  C1H2O2_DIOXI 7.89776E-16  C3H6_2        1.00000E-30
 C1O2          1.23318E-01  C2H4O2_DIOXE 2.01441E-16  C3H8          1.00000E-30
 H1O1          8.75416E-02  C2H1          8.90128E-17  C4            1.00000E-30
 H2            7.66421E-02  C3O2          8.72854E-17  C4H1          1.00000E-30
 O2            6.61597E-02  C2            1.57926E-17  C4H10_1       1.00000E-30
 H             5.95648E-02  C2H2O1        2.52006E-18  C4H10_2       1.00000E-30
 O             4.10215E-02  C2H3          2.72421E-19  C4H4          1.00000E-30
 H1O2          4.23652E-05  C2H4O1_ACETA 1.22338E-20  C4H8_3        1.00000E-30
 H2O2          1.60621E-06  C2H4          1.12569E-20  C4H8_4        1.00000E-30
 C1H1O1        9.35001E-07  C2H4O2_ACETI 7.63780E-21  C4H4_1_3      1.00000E-30
 C1H1O2        6.80303E-07  C3H1          9.69078E-23  C4H6_1        1.00000E-30
 O3            3.01117E-08  C3            6.40718E-23  C4H6_2        1.00000E-30
 C1H2O2_CIS    1.60525E-08  C2H4O1_OXIRA 1.10475E-23  C4H6_3        1.00000E-30
 C1H2O2_TRANS 8.97447E-09  C2H5          2.16226E-24  C4H6_4        1.00000E-30
 C1H2O1        7.25649E-09  C2H6          2.32622E-26  C4H8_5        1.00000E-30
 C             5.41873E-11  C2H6O1        6.30758E-27  C4H6_5        1.00000E-30
 C1H1          5.71254E-12  C2H6O2        8.45966E-28  C5            1.00000E-30
 C1H2          2.82663E-12  C3H4_2        5.35880E-28  C60           1.00000E-30
 C1H3          2.09024E-12  C3H4_1        2.87874E-28  C4H8          1.00000E-30
 C2O1          1.16876E-12  C4H2          6.54217E-30  C6H6          1.00000E-30
 C1H3O1_CH2OH 8.94189E-13  C2H4O3_124TR 4.16521E-30  C6H6O1        1.00000E-30
 C1H4          1.80323E-13  C4H8_2        1.00000E-30  C4H8_1        1.00000E-30
 C1H3O1_CH3O   1.92500E-14  C2H4O3_123TR 1.00000E-30
 C1H4O1        9.77415E-15  C3H6          1.00000E-30
POLY_3: @@ The adiabatic temperature is
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=3103.3954
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Now calculate how the adiabatic temperature varies with
POLY_3: @@ the amount of oxygen
POLY_3: s-a-v 1 n(o) 5 10
   ... the command in full is SET_AXIS_VARIABLE
Increment /.125/:
POLY_3: save tcex22 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    9.00000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    9.00000     for:
     GAS
 Global test at  1.00000E+01 .... OK
 Terminating at    10.0000
 Calculated    11 equilibria

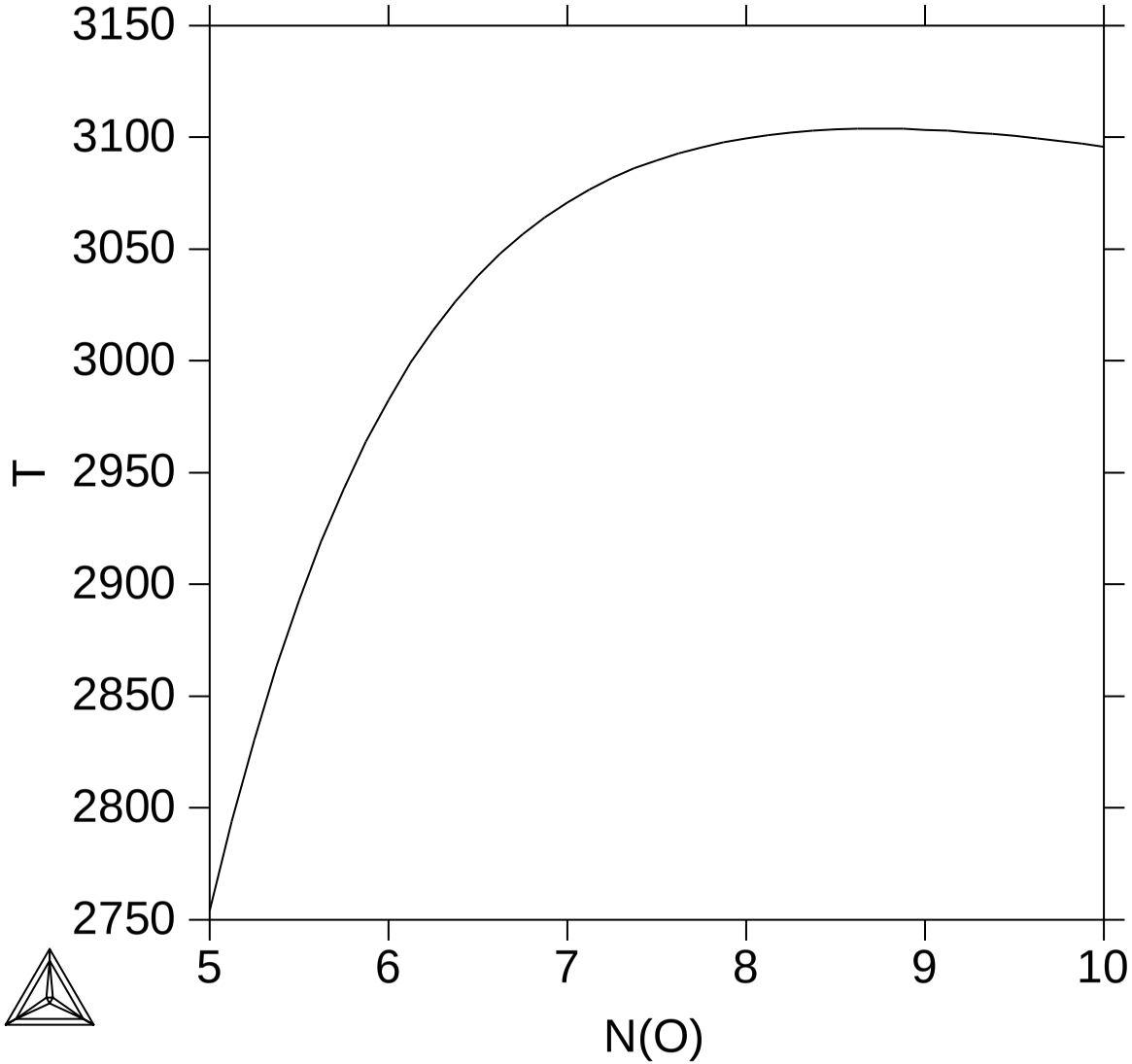
 Phase Region from    9.00000     for:
     GAS
```

```
 Global test at  8.00000E+00 .... OK
 Global test at  6.75000E+00 .... OK
 Global test at  5.50000E+00 .... OK
 Terminating at    5.00000
 Calculated    35 equilibria
 *** Buffer saved on file: tcex22.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

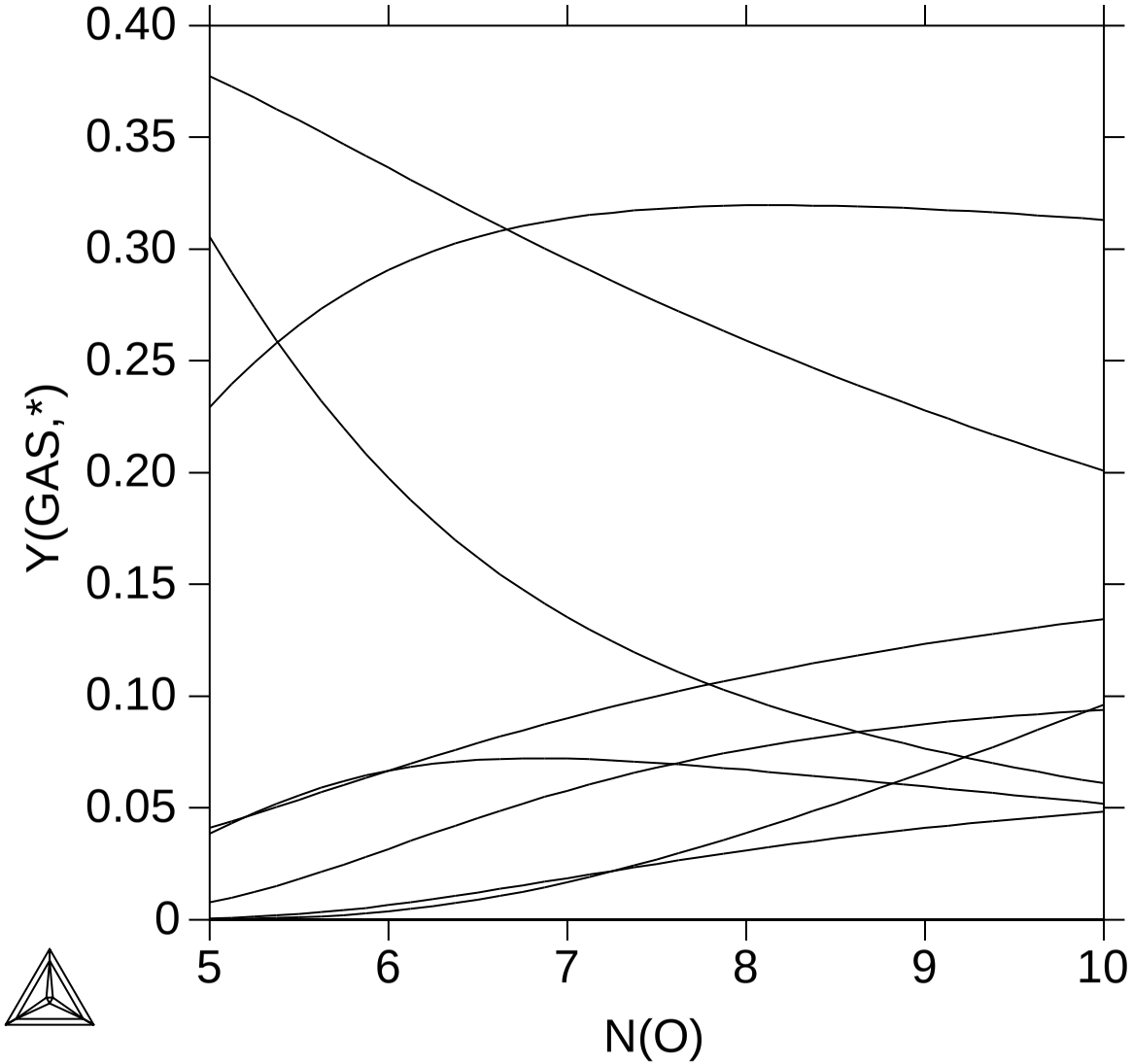
POST:
POST: s-d-a x n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Plot how the gas constitition changes
POST: s-d-a y y(gas,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 22b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Add labels and logarithmic fraction scale
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-s y n 1e-12 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 22c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Plot how the oxygen partial pressure changes
POST: s-d-a y acr(o2,gas)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Plot how the activies of the components change with temperature
POST: @@ Note that the oxygen content changes also ...
POST: @@ We must set reference states
POST: set-ref-state o gas * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state h gas * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state c c_s * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: s-d-a x t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty y lin
   ... the command in full is SET_AXIS_TYPE
POST: s-d-a z n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 5 10
   ... the command in full is SET_SCALING_STATUS
POST: s-d-a y acr(*)
   ... the command in full is SET_DIAGRAM_AXIS
```

```
COLUMN NUMBER /*/:
POST: set-title example 22e
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           3  seconds
```

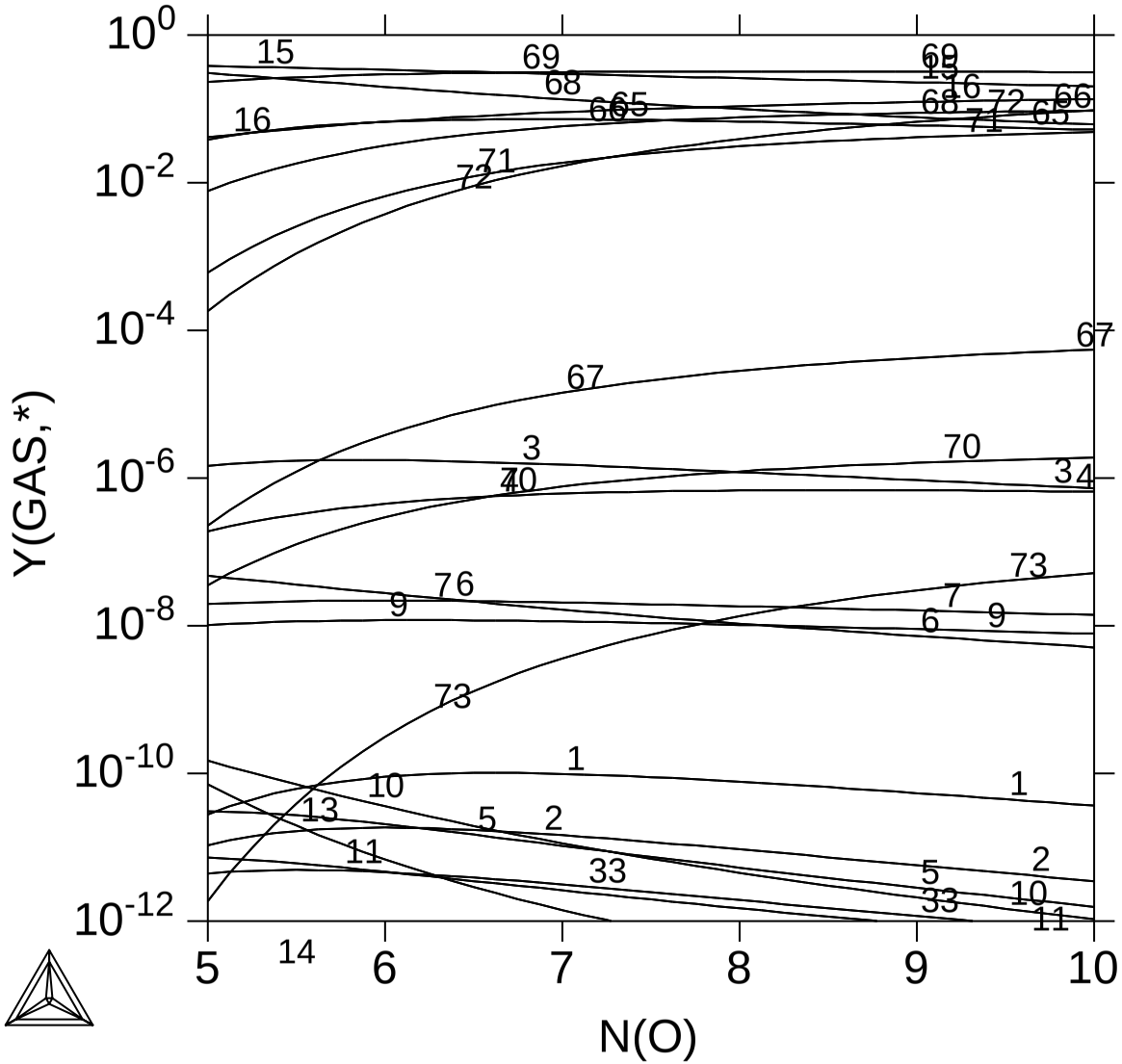
THERMO-CALC (2009.04.15:03.03) :example 22a
DATABASE:SSUB4
P=1E5, N(C)=3., N(H)=8., H=H298;



THERMO-CALC (2009.04.15:03.03) :example 22b
DATABASE:SSUB4
P=1E5, N(C)=3., N(H)=8., H=H298;

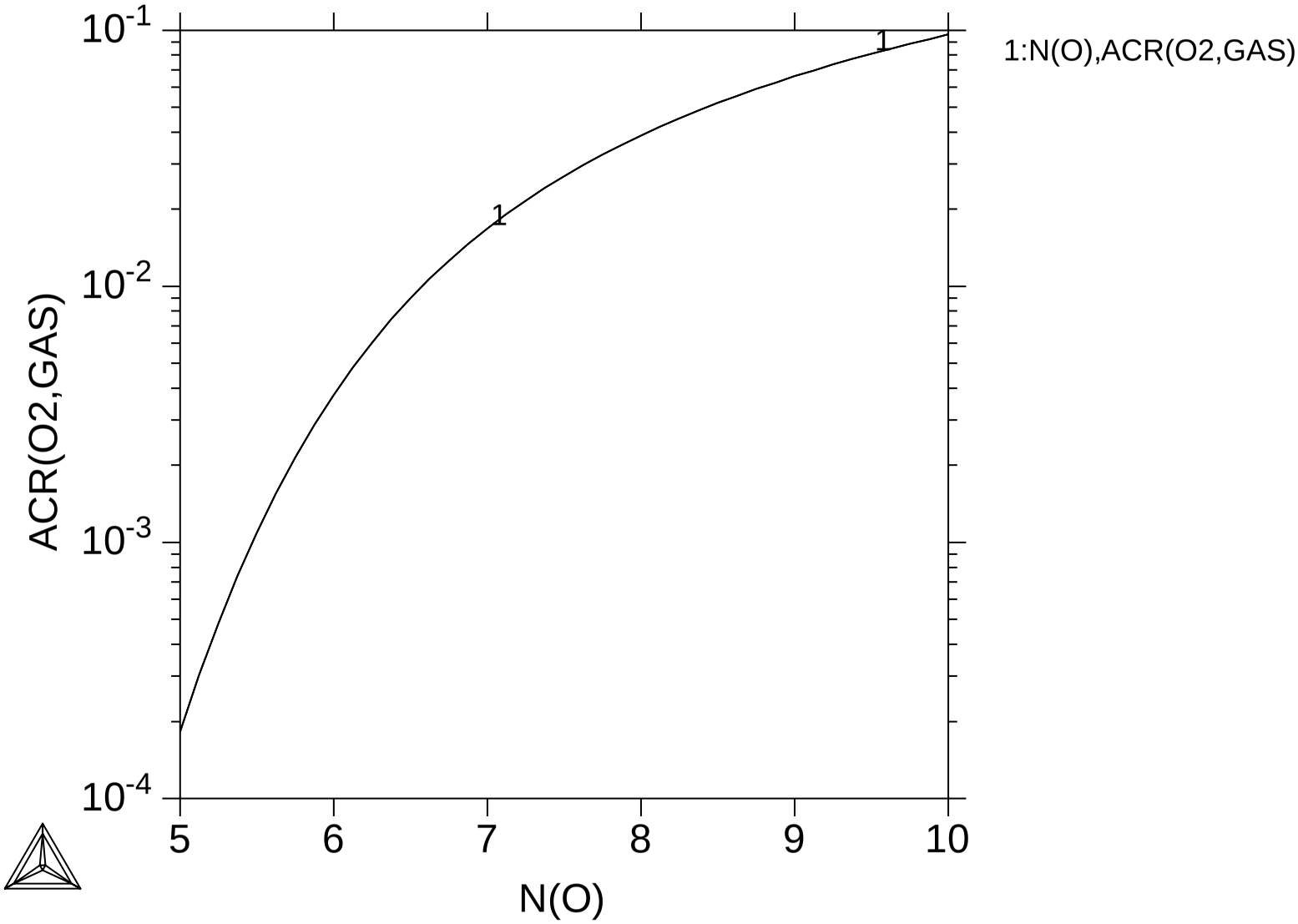


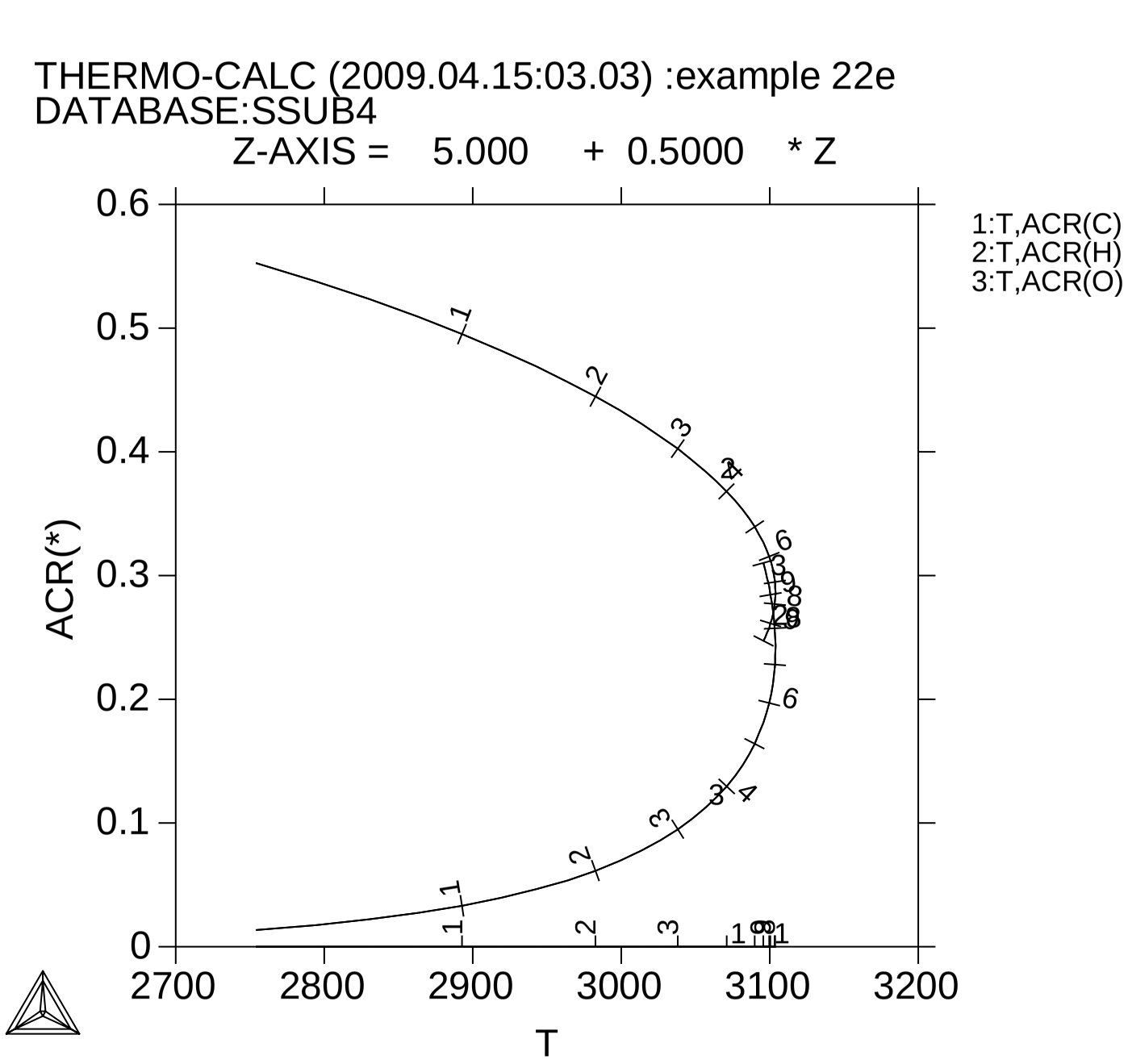
THERMO-CALC (2009.04.15:03.03) :example 22c
DATABASE:SSUB4
P=1E5, N(C)=3., N(H)=8., H=H298;



1:N(O),Y(GAS,C)
2:N(O),Y(GAS,C1H1)
3:N(O),Y(GAS,C1H1O1)
4:N(O),Y(GAS,C1H1O2)
5:N(O),Y(GAS,C1H2)
6:N(O),Y(GAS,C1H2O1)
7:N(O),Y(GAS,C1H2O2_CIS)
9:N(O),Y(GAS,C1H2O2_TRANS)
10:N(O),Y(GAS,C1H3)
11:N(O),Y(GAS,C1H3O1_CH2OH)
15:N(O),Y(GAS,C1O1)
16:N(O),Y(GAS,C1O2)
33:N(O),Y(GAS,C2O1)
65:N(O),Y(GAS,H)
66:N(O),Y(GAS,H1O1)
67:N(O),Y(GAS,H1O2)
68:N(O),Y(GAS,H2)
69:N(O),Y(GAS,H2O1)
70:N(O),Y(GAS,H2O2)
71:N(O),Y(GAS,O)
72:N(O),Y(GAS,O2)
73:N(O),Y(GAS,O3)
13:N(O),Y(GAS,C1H4)
14:N(O),Y(GAS,C1H4O1)

THERMO-CALC (2009.04.15:03.03) :example 22d
DATABASE:SSUB4
P=1E5, N(C)=3., N(H)=8., H=H298;




THERMO-CALC (2009.04.15:03.03) :example 22e
DATABASE:SSUB4
Z-AXIS = 5.000 + 0.5000 * Z
1:T,ACR(C)
2:T,ACR(H)
3:T,ACR(O)
ACR(*)
T
0.6
0.5
0.4
0.3
0.2
0.1
0
2700
2800
2900
3000
3100
3200

23

Calculation of a para-equilibrium and the T_0 temperature

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of T-zero and paraequilibria in a low alloyed steel
SYS: @@
SYS: set-log ex23,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ Define the material
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/:  tcfe6
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:  Y
1st alloying element: mn 1.5
2nd alloying element: si .3
Next alloying element: c .3
Next alloying element:
Temperature (C) /1000/:  700
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED

 This database has following phases for the defined system

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    KSI_CARBIDE             A1_KAPPA
 KAPPA                   FE4N_LP1                FECN_CHI
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 AL4C3                   FE8SI2C                 SIC

Reject phase(s) /NONE/:  NONE
Restore phase(s): /NONE/:  NONE
 ..................................................

    The following phases are retained in this system:

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    KSI_CARBIDE             A1_KAPPA
 KAPPA                   FE4N_LP1                FECN_CHI
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 AL4C3                   FE8SI2C                 SIC
```

```
 ..................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'J. Grobner, H.L. Lukas and F. Aldinger, Calphad, 20 (1996), 247-254; Si-C
      and Al-Si-C'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
                    :
                    :
                    :
  'Thermo-Calc Software (2008): Volume data updated for TCFE6 database (TCFE
      v6, April, 2008).'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'Estimated parameter for solubility of C in Fe4N, 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'B.-J. Lee, KRISS, unpublished research, during 1993-1995'
  'I. Ansara, unpublished work (1991); Cr-Si'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
 Calculated        11055  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    973.15 K (   700.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50671E+01
 Total Gibbs energy -4.16088E+04,  Enthalpy  2.38836E+04,  Volume  7.24185E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3754E-02  3.0000E-03 2.2665E-01 -1.2010E+04 SER
 FE                      9.6533E-01  9.7900E-01 6.6031E-03 -4.0620E+04 SER
 MN                      1.5035E-02  1.5000E-02 6.5723E-05 -7.7919E+04 SER
 SI                      5.8820E-03  3.0000E-03 2.1018E-10 -1.8030E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.4142E-01, Mass 4.1252E+01, Volume fraction 7.4788E-01  Mass fractions:
 FE  9.87818E-01  MN  8.85142E-03  SI  3.22070E-03  C   1.10187E-04

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 2.5248E-01, Mass 1.3742E+01, Volume fraction 2.4758E-01  Mass fractions:
 FE  9.57752E-01  MN  3.35378E-02  C   6.35700E-03  SI  2.35347E-03

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 6.1027E-03, Mass 7.3300E-02, Volume fraction 4.5452E-03  Mass fractions:
 C   1.00000E+00  SI  0.00000E+00  MN  0.00000E+00  FE  0.00000E+00
POLY_3: @@ Suspend some phases that normally never appear
POLY_3: ch-st p gra m5c2=sus
```

```
   ... the command in full is CHANGE_STATUS
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Set axis for T-w(c) phase diagram
POLY_3: s-a-v 1 w(c)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  .01
Increment /2.5E-04/:  2.5E-04
POLY_3: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  800
Max value /1/:  1200
Increment /10/:  30
POLY_3: save tcex23a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Working hard

 Phase region boundary   1 at:   2.500E-04  9.455E+02
     BCC_A2
     CEMENTITE
  ** FCC_A1
 *** Buffer saved on file: tcex23a.POLY3
 Calculated.            2  equilibria

 Phase region boundary   2 at:   6.694E-05  9.437E+02
     BCC_A2
  ** CEMENTITE
  ** FCC_A1

 Phase region boundary   3 at:   6.694E-05  9.437E+02
     BCC_A2
  ** FCC_A1
```

```
 Calculated           14  equilibria

 Phase region boundary   4 at:   6.694E-05  9.437E+02
    BCC_A2
  ** CEMENTITE
 Calculated..           10  equilibria
 Terminating at axis limit.

       :
       :
       :

 Phase region boundary  26 at:   6.583E-03  9.981E+02
  ** BCC_A2
    FCC_A1
 Calculated           38  equilibria

 Phase region boundary  27 at:   6.583E-03  9.981E+02
  ** BCC_A2
    FCC_A1
 Calculated.            3  equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   9.750E-03  1.095E+03
  ** CEMENTITE
    FCC_A1
 Calculated.           12  equilibria
 Terminating at known equilibrium

 Phase region boundary  29 at:   9.750E-03  1.095E+03
  ** CEMENTITE
    FCC_A1
 Calculated..           3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: tcex23a.POLY3
 CPU time for mapping          11  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,
POST:
POST:
POST: set-title example 23a
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Add labels
POST: add
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .005
Give Y coordinate in axis units: 1100
Automatic phase labels? /Y/:  Y
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated        10917  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
 Stable phases are: FCC_A1
Text size: /.3999999762/:  .34
POST: add
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .003
Give Y coordinate in axis units: 850
Automatic phase labels? /Y/:  Y
 Automatic labelling not always possible
 Using global minimization procedure
 Calculated        10917  grid points in            0  s
```

```
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_A2+CEMENTIT
Text size: /.3999999762/:  .34
POST: set-title example 23b
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /A/:  ?
 THE OPTIONS MEANS:
 A     LIST STABLE PHASES ALONG LINE
 B     AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
 C     LIST AXIS QUANTITIES
 D     AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
 E     AS B WITH CHANGING COLORS
 F     AS D WITH CHANGING COLORS
 N     NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /A/:  e
POST: set-title example 23c
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: ba
   ... the command in full is BACK
POLY_3: @@ Now calculate the T-zero temperature for the steel
POLY_3: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY_3: advanced-options
Which option? /STEP_AND_MAP/:  ?
 EQUILIBRIUM_CALCUL       OUTPUT_FILE_FOR_SHOW     STABILITY_CHECK
 GLOBAL_MINIMIZATION      PARAEQUILIBRIUM          STEP_AND_MAP
 LIST_PHASE_ADDITION      PHASE_ADDITION           T-ZERO TEMPERATURE
 MAJOR_CONSTITUENTS       PRESENT_PHASE            TOGGLE_ALTERNATE_MODE
 NEW_COMPOSITION_SET      SHOW_FOR_T=
Which option? /STEP_AND_MAP/:  t-z
This command calculates the temperature when two phases have the same Gibbs
energy.  You must calculate an equilibrium at an estimated temperature first.
Name of first phase: fcc
Name of second phase: bcc
 The T0 temperature is  922.21 K
 Note: LIST-EQUILIBRIUM is not relevant
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Calculate the T-zero line, remove the T-axis
POLY_3: l-ax
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(C)                 Min: 0         Max: 1E-2      Inc: 2.5E-4
  Axis No 2: T                    Min: 800       Max: 1200      Inc: 30
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex23b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  ?
 The following options are available:
 NORMAL             Stepping with given conditions
 INITIAL_EQUILIBRIA An initial equilibrium stored at every step
 EVALUATE           Specified variables evaluated after each step
 SEPARATE_PHASES    Each phase calculated separately
 T-ZERO             T0 line calculation
 PARAEQUILIBRIUM    Paraequilibrium diagram
 MIXED_SCHEIL       Scheil with fast diffusing elements
 ONE_PHASE_AT_TIME  One phase at a time
Option? /NORMAL/:  t-z
Name of first phase: fcc
Name of second phase: bcc
 Phase Region from   0.300000E-02 for:
     BCC_A2
```

```
     FCC_A1
   3.000000E-03         922.21
   2.750000E-03         932.54
   2.500000E-03         943.23
   2.250000E-03         954.34
   2.000000E-03         965.98
   1.750000E-03         978.31
   1.500000E-03         991.57
   1.250000E-03        1006.14
   1.000000E-03        1022.76
   7.500000E-04        1041.59
   5.000000E-04        1062.86
   2.500000E-04        1087.12
   2.500000E-10        1115.11

 Phase Region from   0.167112E-02 for:
     BCC_A2
     FCC_A1
   1.671124E-03         982.32
   1.921124E-03         969.73
   2.171124E-03         957.89
   2.421124E-03         946.63
   2.671124E-03         935.82
   2.921124E-03         925.38
   3.171124E-03         915.26
   3.421124E-03         905.40
   3.671124E-03         895.77
   3.921124E-03         886.33
   4.171124E-03         877.06
   4.421124E-03         867.93
   4.671124E-03         858.95
   4.921124E-03         850.07
   5.171124E-03         841.30
   5.421124E-03         832.63
   5.671124E-03         824.03
   5.921124E-03         815.51
   6.171124E-03         807.06
   6.421124E-03         798.67
   6.671124E-03         790.33
   6.921124E-03         782.04
   7.171124E-03         773.79
   7.421124E-03         765.58
   7.671124E-03         757.40
   7.921124E-03         749.26
   8.171124E-03         741.14
   8.421124E-03         733.04
   8.671124E-03         724.96
   8.921124E-03         716.90
   9.171124E-03         708.85
   9.421124E-03         700.82
   9.671124E-03         692.79
   9.921124E-03         684.77
   1.000000E-02         682.24
 *** Buffer savend on file tcex23b.POLY3
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-p-f ##1,,,,,,
POST:
POST:
POST: set-title example 23d
POST: s-d-a x w(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ write the line on a data file
POST: make tcex23b y
```

```
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: ba
   ... the command in full is BACK
POLY_3: @@ plot together with phase diagram
POLY_3: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,
POST: set-title example 23e
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: a-e-d y tcex23b
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  1
POST: set-title example 23f
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: ba
   ... the command in full is BACK
POLY_3: @@ Now calculate the para-equilibrium for the steel
POLY_3: @@ At paraequilibrium only C is mobile, the other alloying elements have
POLY_3: @@ the same compositions in both phases
POLY_3: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        10917  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    973.15 K (   700.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50671E+01
 Total Gibbs energy -4.16068E+04,  Enthalpy  2.38034E+04,  Volume  7.22424E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3754E-02  3.0000E-03 2.3682E-01 -1.1655E+04 SER
 FE                      9.6533E-01  9.7900E-01 6.6051E-03 -4.0617E+04 SER
 MN                      1.5035E-02  1.5000E-02 6.2466E-05 -7.8331E+04 SER
 SI                      5.8820E-03  3.0000E-03 2.1440E-10 -1.8014E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.6441E-01, Mass 4.2529E+01, Volume fraction 7.7288E-01  Mass fractions:
 FE  9.88221E-01  MN  8.40073E-03  SI  3.26359E-03  C   1.14706E-04

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 2.0669E-01, Mass 1.1242E+01, Volume fraction 2.0306E-01  Mass fractions:
 FE  9.59011E-01  MN  3.21007E-02  C   6.54001E-03  SI  2.34865E-03

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.8906E-02, Mass 1.2957E+00, Volume fraction 2.4065E-02  Mass fractions:
 FE  8.49786E-01  MN  8.32277E-02  C   6.69864E-02  SI  0.00000E+00
POLY_3: advance para
   ... the command in full is ADVANCED_OPTIONS
```

```
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/:  c
Fast diffusing component: /NONE/:
 NP(FCC) =   0.4280 with U-fractions C  =  3.17220E-02
 NP(BCC) =   0.5720 with U-fractions C  =  6.47538E-04
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3:
POLY_3: @@ Now calculate the para-equilibrium for the steel at varying temperatures
POLY_3: s-a-v 1 t 800 1200 20
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex23c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step para
   ... the command in full is STEP_WITH_OPTIONS

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/:  c
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in    phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    973.150     for:
     BCC_A2
     FCC_A1
   9.731500E+02    0.428    0.572   3.172200E-02   6.475377E-04  -1.290452E+00
   9.531500E+02    0.345    0.655   3.908052E-02   7.297760E-04  -8.659516E-01
   9.331500E+02    0.285    0.715   4.699458E-02   8.039957E-04  -4.522834E-01
   9.131500E+02    0.240    0.760   5.535054E-02   8.679372E-04  -4.631426E-02
   8.931500E+02    0.206    0.794   6.405501E-02   9.201210E-04   3.549783E-01
   8.731500E+02    0.180    0.820   7.303132E-02   9.596491E-04   7.543208E-01
   8.531500E+02    0.160    0.840   8.221743E-02   9.860983E-04   1.154160E+00
   8.331500E+02    0.143    0.857   9.156332E-02   9.994314E-04   1.556708E+00
   8.131500E+02    0.129    0.871   1.010286E-01   9.999336E-04   1.963997E+00
   8.000000E+02    0.122    0.878   1.073012E-01   9.935324E-04   2.235299E+00

 Phase Region from    973.150     for:
     BCC_A2
     FCC_A1
   9.731500E+02    0.429    0.571   3.168117E-02   6.465368E-04  -1.292139E+00
   9.931500E+02    0.547    0.453   2.501532E-02   5.595693E-04  -1.730355E+00
   1.013150E+03    0.720    0.280   1.919684E-02   4.725723E-04  -2.182535E+00
   1.033150E+03    0.977    0.023   1.426175E-02   3.879729E-04  -2.653059E+00
   1.053150E+03    1.411   -0.411   9.973814E-03   3.003908E-04  -3.172815E+00
   1.073150E+03    2.275   -1.275   6.247344E-03   2.085287E-04  -3.792875E+00
   1.093150E+03    4.762   -3.762   3.016699E-03   1.116447E-04  -4.664306E+00
   1.113150E+03   64.105  -63.105   2.267080E-04   9.302453E-06  -7.388093E+00
 *** Buffer savend on file tcex23c.POLY3

 *** ERROR     7 IN NS01AD
 *** Numerical error
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,,
POST:
POST:
POST: set-title example 23g
```

POST: **s-d-a x x(*,c)**
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: **s-d-a y t-k**
... the command in full is SET_DIAGRAM_AXIS
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **s-d-a x w(*,c)**
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: **s-t-s 3**
... the command in full is SET_TIELINE_STATUS
POST: **set-title example 23h**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **make tcex23c y**
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: **ba**
... the command in full is BACK
POLY_3: **read tcex23a**
... the command in full is READ_WORKSPACES
POLY_3: **po**
... the command in full is POST

POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

POST: **s-p-f ##1,,,,,,,,,**
POST:
POST:
POST: **set-title example 23i**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **a-e-d y tcex23c**
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: **0**
DATASET NUMBER(s): /-1/: **1**
POST: **set-title example 23j**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **a-e-d y tcex23b.exp tcex23c.exp 0; 1; 0; 1;**
... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: **set-title example 23k**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **ba**
... the command in full is BACK
POLY_3: ***@@ Now calculate both a normal and para-equilibrium for the steel at 1000 K***
POLY_3: ***@@ Note that a para equilibrium does not always exist for the given conditions***
POLY_3: ***@@ The calculated results are the amounts of the two phases.***
POLY_3: ***@@ This indicates how much of the phases that can be tranformed***
POLY_3: ***@@ at para-equilibrium conditions.***
POLY_3: ***@@ The carbon content of the phases are also listed,***
POLY_3: ***@@ the other alloying elements have the same fractions in both phases***
POLY_3: **read tcex23a.POLY3**
... the command in full is READ_WORKSPACES

```
POLY_3: s-c T=1000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        10917  grid points in            1  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=1000, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.50671E+01
 Total Gibbs energy -4.34548E+04,  Enthalpy  2.63172E+04,  Volume  7.20607E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3754E-02  3.0000E-03 1.6744E-01 -1.4859E+04 SER
 FE                      9.6533E-01  9.7900E-01 6.1057E-03 -4.2392E+04 SER
 MN                      1.5035E-02  1.5000E-02 4.1161E-05 -8.3960E+04 SER
 SI                      5.8820E-03  3.0000E-03 3.4194E-10 -1.8123E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.3820E-01, Mass 2.9381E+01, Volume fraction 5.3141E-01  Mass fractions:
 FE  9.69754E-01  MN  2.22121E-02  C   5.51915E-03  SI  2.51464E-03

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.6180E-01, Mass 2.5686E+01, Volume fraction 4.6859E-01  Mass fractions:
 FE  9.89576E-01  MN  6.75038E-03  SI  3.55518E-03  C   1.18465E-04
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  para
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/:  c
Fast diffusing component: /NONE/:
 NP(FCC) =   0.5982 with U-fractions C  =  2.29562E-02
 NP(BCC) =   0.4018 with U-fractions C  =  5.30475E-04
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Now calculate an isothermal phase diagram at 1000 K
POLY_3: s-a-v 2 w(mn) 0 .1,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: @?<Hit_return_to_continue>
POLY_3: save tcex23d y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
```

```
Generating start point   1
Generating start point   2
Generating start point   3
Generating start point   4
Generating start point   5
Generating start point   6
Generating start point   7
Generating start point   8
Generating start point   9
Generating start point  10
Working hard
Generating start point  11
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28
Generating start point  29
Generating start point  30
Working hard
Generating start point  31
Generating start point  32

Phase region boundary   1 at:   2.585E-03  2.500E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.           11  equilibria

Phase region boundary   2 at:   1.821E-04  1.138E-03
    BCC_A2
 ** CEMENTITE
 ** FCC_A1

Phase region boundary   3 at:   1.821E-04  1.138E-03
    BCC_A2
 ** CEMENTITE
Calculated           14  equilibria

Phase region boundary   4 at:   1.821E-04  1.138E-03
    BCC_A2
 ** FCC_A1
Calculated           28  equilibria

      :
      :
      :

Phase region boundary  38 at:   6.732E-03  9.750E-02
 ** CEMENTITE
    FCC_A1
Calculated.           38  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.732E-03  9.750E-02
 ** CEMENTITE
    FCC_A1
Calculated..           3  equilibria
Terminating at known equilibrium
Terminating at axis limit.
```

```
 Phase region boundary  40 at:   9.750E-03  7.619E-03
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated.           11  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.750E-03  7.619E-03
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated..           3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: tcex23d.POLY3
 CPU time for mapping          10  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,
POST:
POST:
POST: set-title example 23l
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: add .001 .03,,,,
   ... the command in full is ADD_LABEL_TEXT
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_A2+FCC_A1
POST: set-title example 23m
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: ba
   ... the command in full is BACK
POLY_3: @@ Calculate the corresponing para-equilibrium diagram
POLY_3: @@ where fcc and bcc have the same alloy composition.
POLY_3: read tcex23d
   ... the command in full is READ_WORKSPACES
POLY_3: @@ Only one axis is set, the interstitial composition
POLY_3: @@ must not be an axis
POLY_3: s-a-v 1 w(mn) 0 .1,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex23e y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  ?
 The following options are available:
 NORMAL             Stepping with given conditions
 INITIAL_EQUILIBRIA An initial equilibrium stored at every step
 EVALUATE           Specified variables evaluated after each step
 SEPARATE_PHASES    Each phase calculated separately
 T-ZERO             T0 line calculation
 PARAEQUILIBRIUM    Paraequilibrium diagram
 MIXED_SCHEIL       Scheil with fast diffusing elements
 ONE_PHASE_AT_TIME  One phase at a time
Option? /NORMAL/:  para
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
```

```
Name of second phase: bcc
Fast diffusing component: /C/:  c
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in    phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from   0.150000E-01 for:
     BCC_A2
     FCC_A1
   1.500000E-02    0.598    0.402   2.295618E-02   5.304752E-04  -1.881771E+00
   1.250000E-02    0.542    0.458   2.524490E-02   5.935358E-04  -1.753638E+00
   1.000000E-02    0.494    0.506   2.753767E-02   6.587191E-04  -1.633619E+00
   7.500000E-03    0.454    0.546   2.983359E-02   7.260508E-04  -1.520467E+00
   5.000000E-03    0.420    0.580   3.213187E-02   7.955567E-04  -1.413204E+00
   2.500000E-03    0.390    0.610   3.443178E-02   8.672626E-04  -1.311054E+00
   2.500000E-09    0.363    0.637   3.673267E-02   9.411946E-04  -1.213385E+00

 Phase Region from   0.150000E-01 for:
     BCC_A2
     FCC_A1
   1.500000E-02    0.598    0.402   2.295989E-02   5.306073E-04  -1.881370E+00
   1.750000E-02    0.667    0.333   2.067628E-02   4.696395E-04  -2.019223E+00
   2.000000E-02    0.752    0.248   1.839858E-02   4.107379E-04  -2.169018E+00
   2.250000E-02    0.862    0.138   1.612841E-02   3.538881E-04  -2.333767E+00
   2.500000E-02    1.006   -0.006   1.386691E-02   2.990604E-04  -2.517864E+00
   2.750000E-02    1.205   -0.205   1.161307E-02   2.461731E-04  -2.728233E+00
   3.000000E-02    1.501   -0.501   9.357235E-03   1.949519E-04  -2.977273E+00
   3.250000E-02    1.985   -0.985   7.097179E-03   1.453158E-04  -3.286868E+00
   3.500000E-02    2.925   -1.925   4.831565E-03   9.721155E-05  -3.704636E+00
   3.750000E-02    5.540   -4.540   2.558996E-03   5.058863E-05  -4.373542E+00
   4.000000E-02   51.139  -50.139   2.780008E-04   5.399171E-06  -6.626764E+00
 *** Buffer savend on file tcex23e.POLY3

 *** ERROR     8 IN NS01AD
 *** Numerical error
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

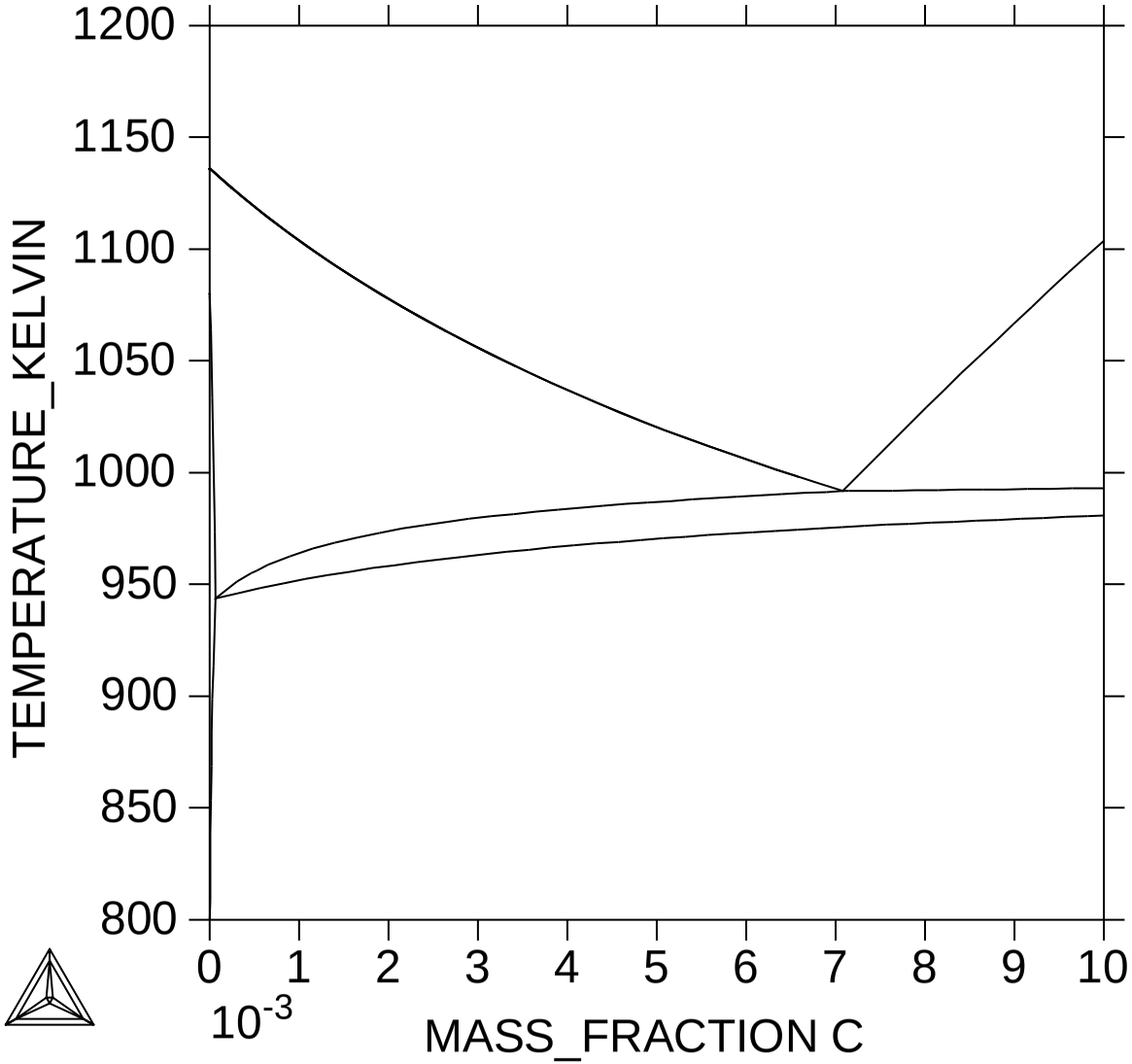
POST: s-p-f ##1,,,,,,
POST:
POST:
POST: s-t-s 3
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 23n
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: set-title example 23o
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: make tcex23e y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: @?<Hit_return_to_continue>
POST: ba
   ... the command in full is BACK
POLY_3: @@ Now overlay the two diagrams
POLY_3: read tcex23d
   ... the command in full is READ_WORKSPACES
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01
```

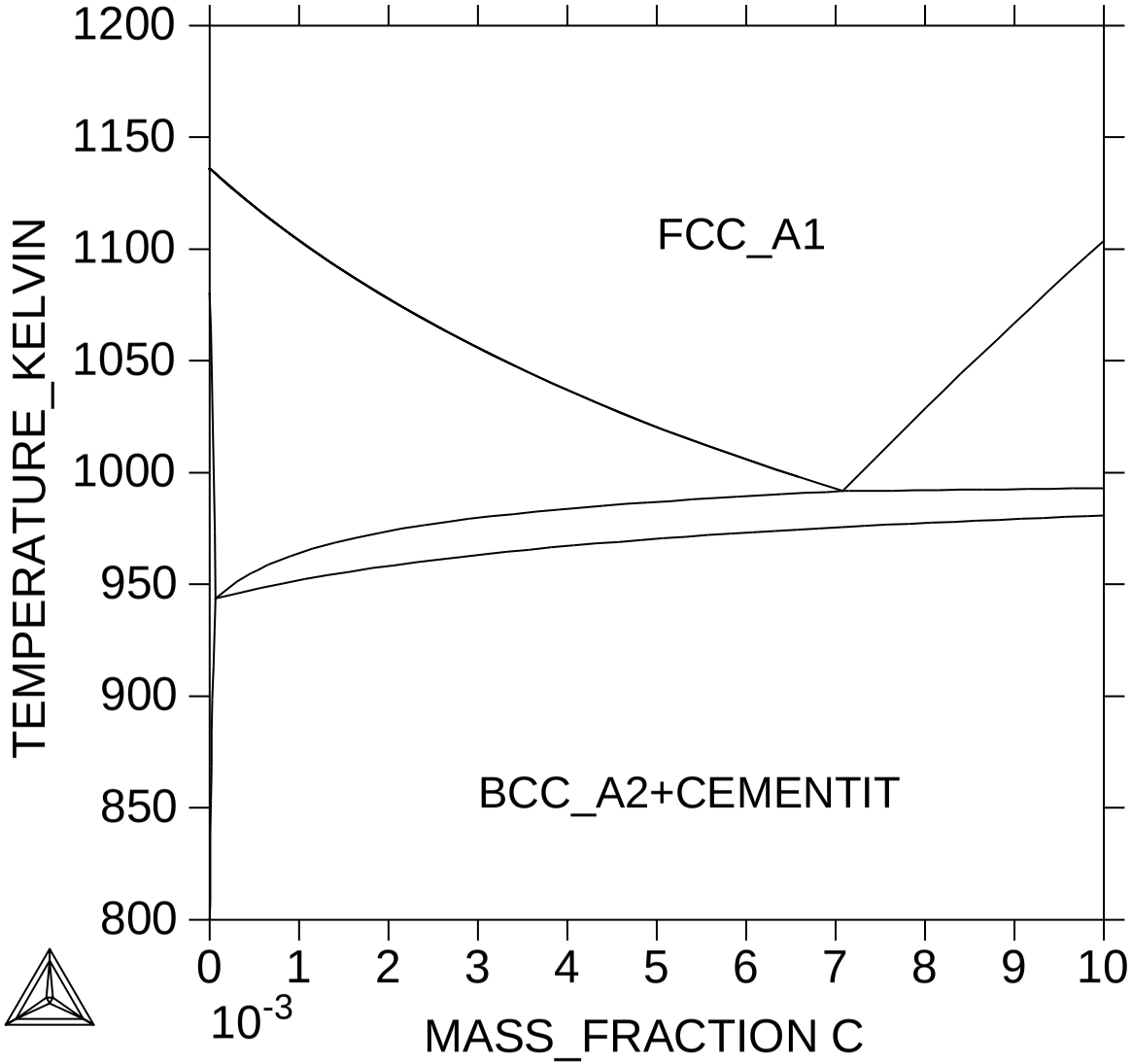
```
 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,
POST:
POST:
POST: set-title example 23p
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: a-e-d y tcex23e
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  1
POST: set-title example 23q
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
 CPU time           37  seconds
```

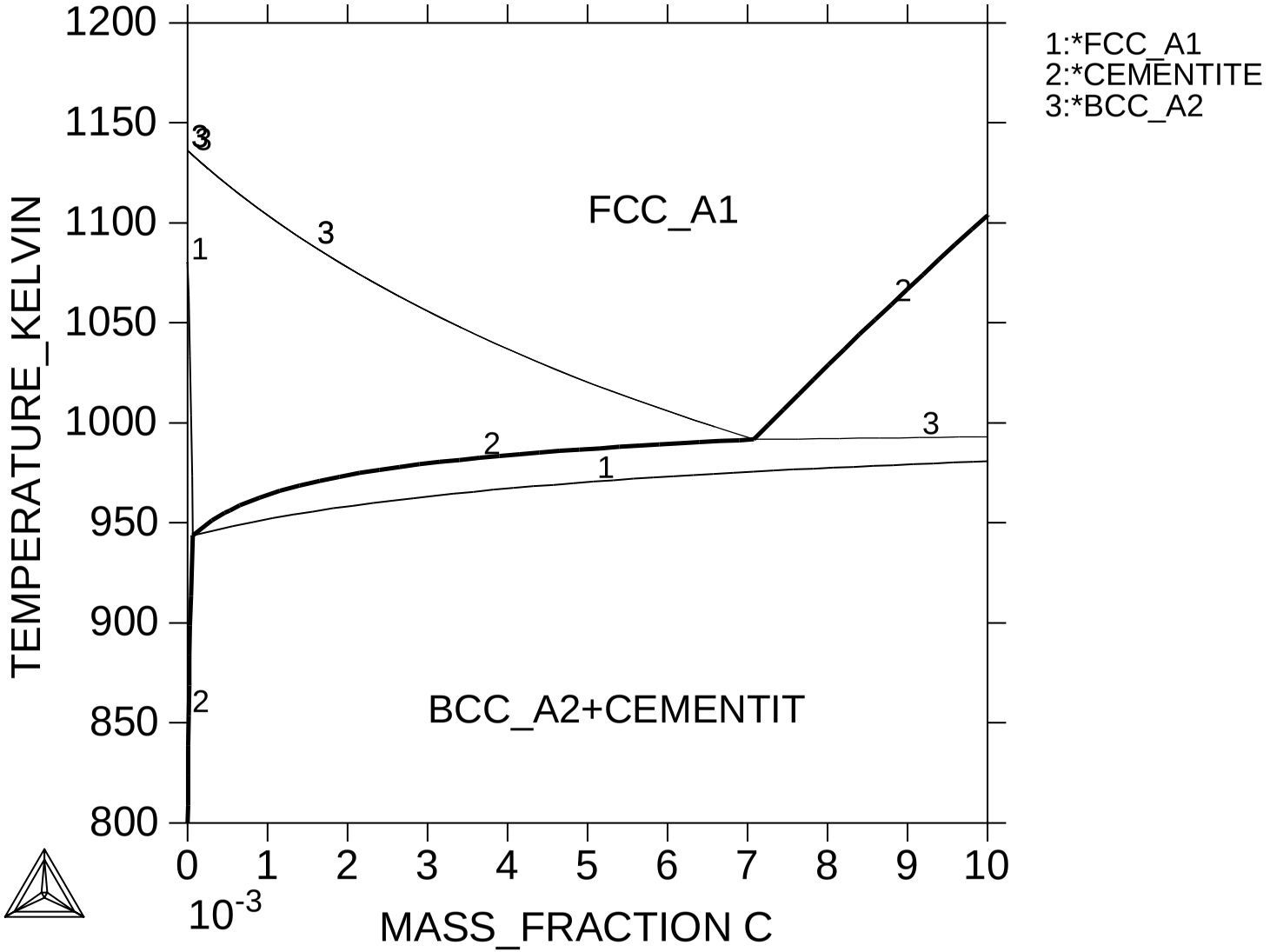
THERMO-CALC (2009.04.15:03.03) :example 23a
DATABASE:TCFE6
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1;



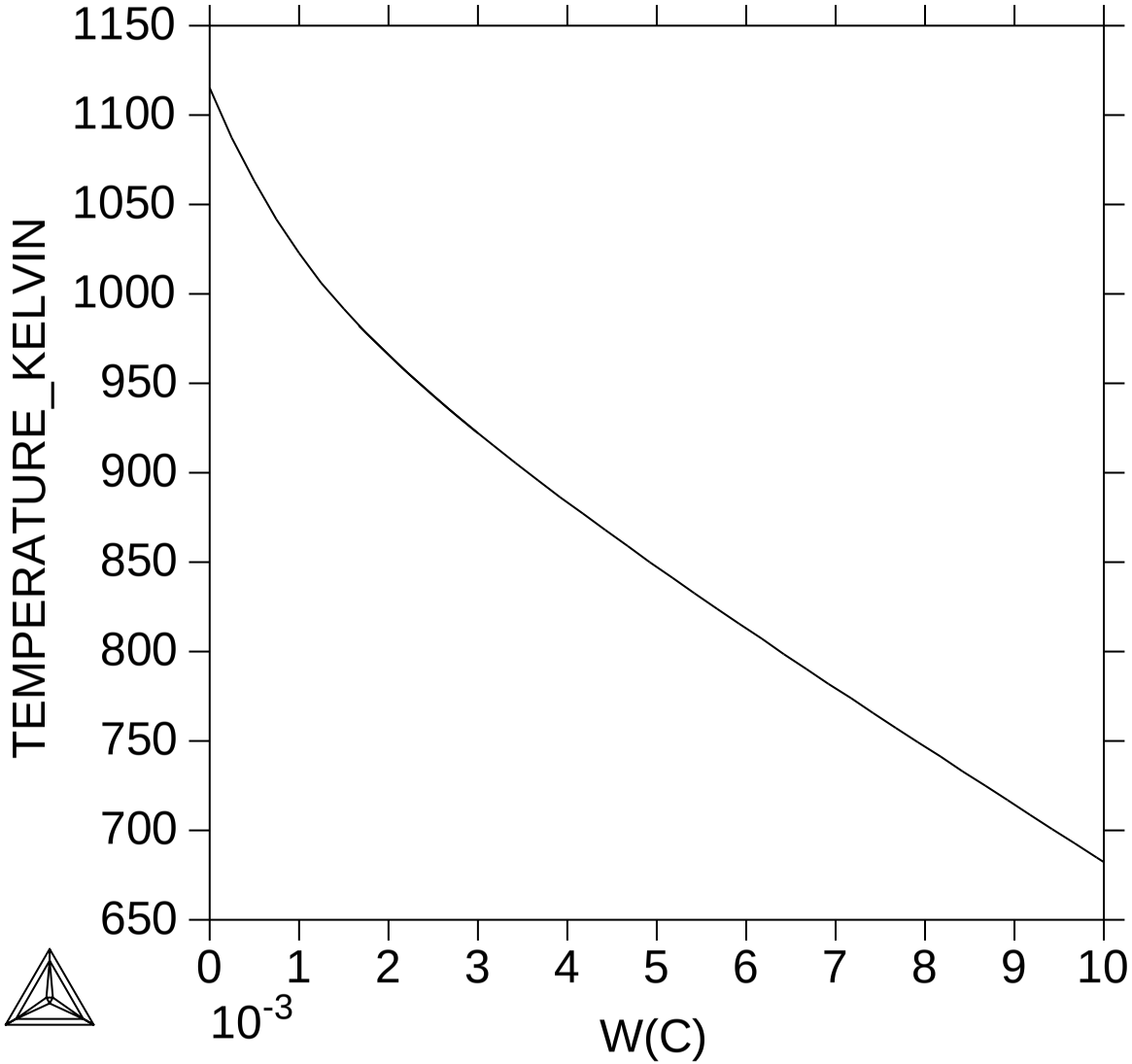
THERMO-CALC (2009.04.15:03.03) :example 23b
DATABASE:TCFE6
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1;



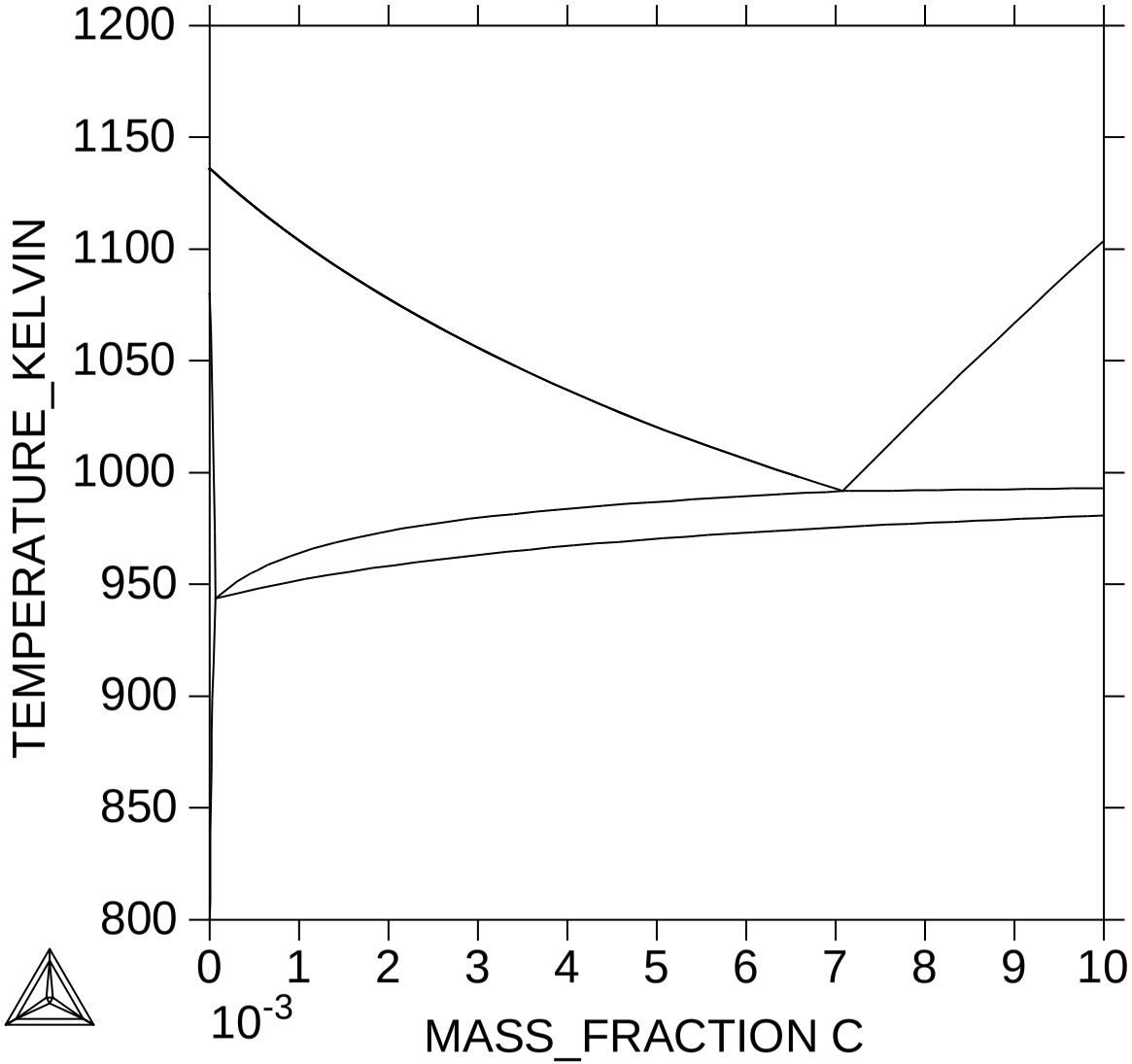
THERMO-CALC (2009.04.15:03.03) :example 23c
DATABASE:TCFE6
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1;

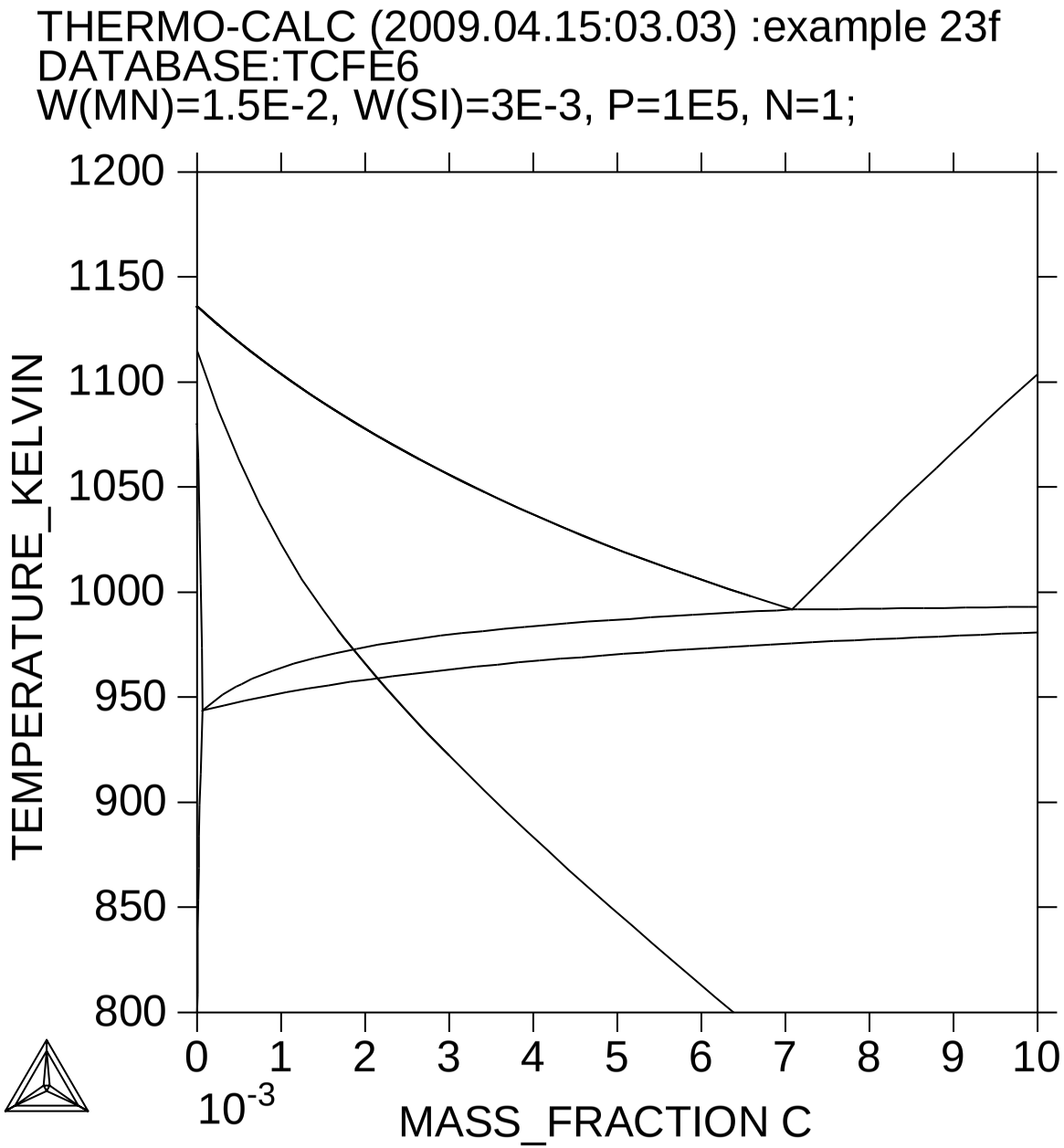


THERMO-CALC (2009.04.15:03.03) :example 23d
DATABASE:TCFE6
T=682.239, W(MN)=1.502E-2, W(SI)=3.004E-3, P=1E5, N=0.993897;

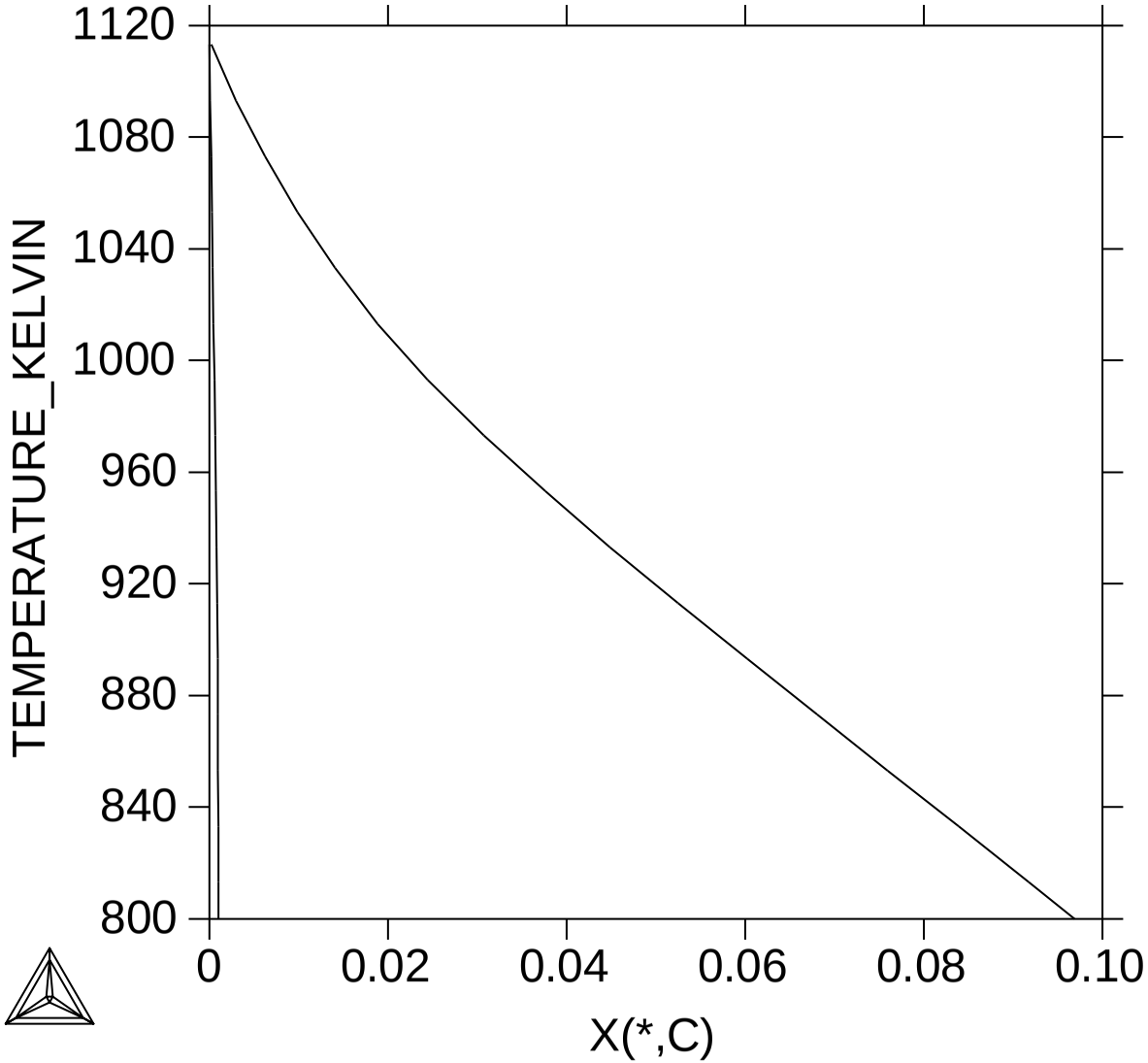


THERMO-CALC (2009.04.15:03.03) :example 23e
DATABASE:TCFE6
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1;

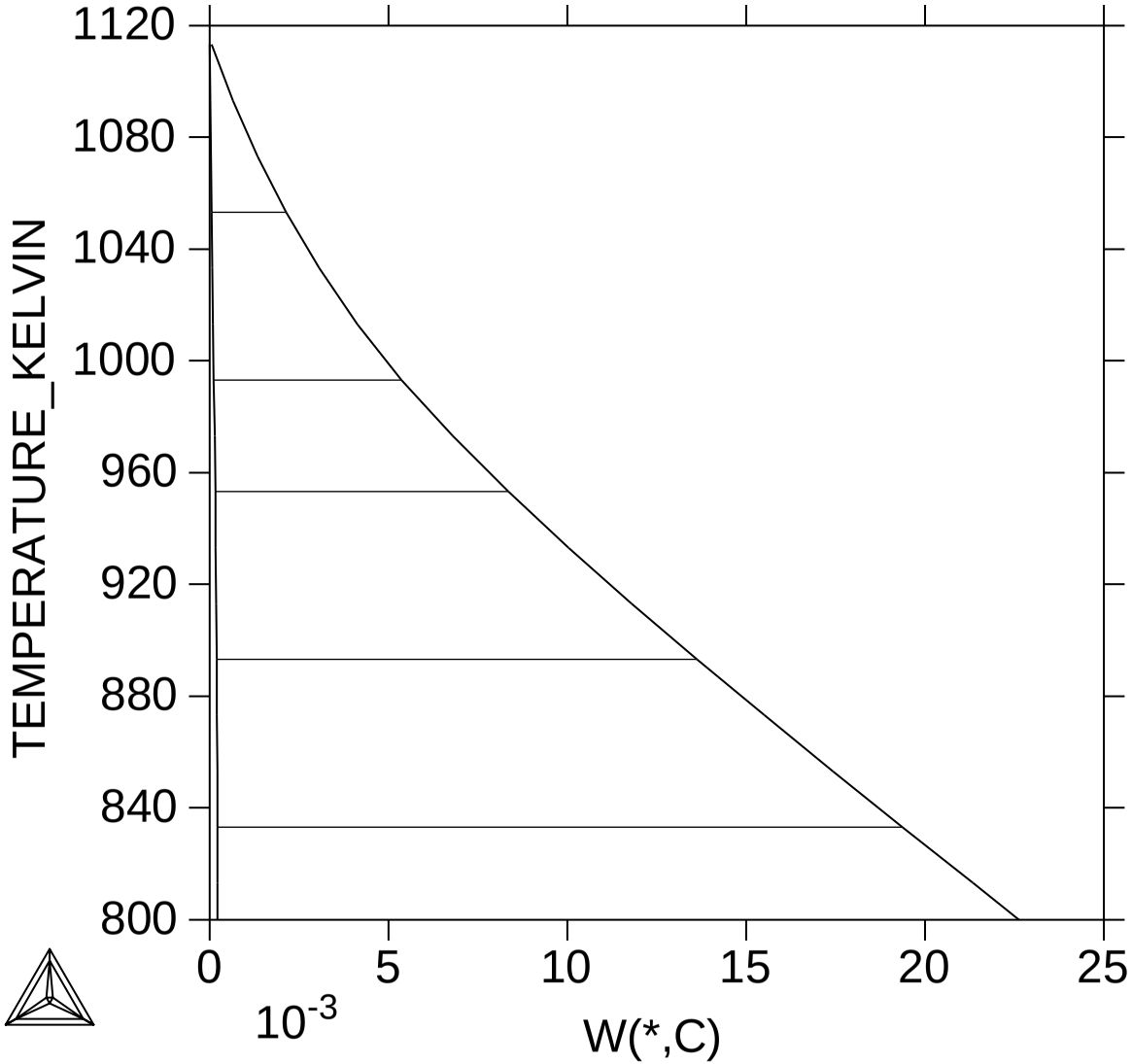



THERMO-CALC (2009.04.15:03.03) :example 23f
DATABASE:TCFE6
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1;
1200
1150
1100
1050
1000
950
900
850
800
TEMPERATURE_KELVIN
0
1
2
3
4
5
6
7
8
9
10
10-3
MASS_FRACTION C

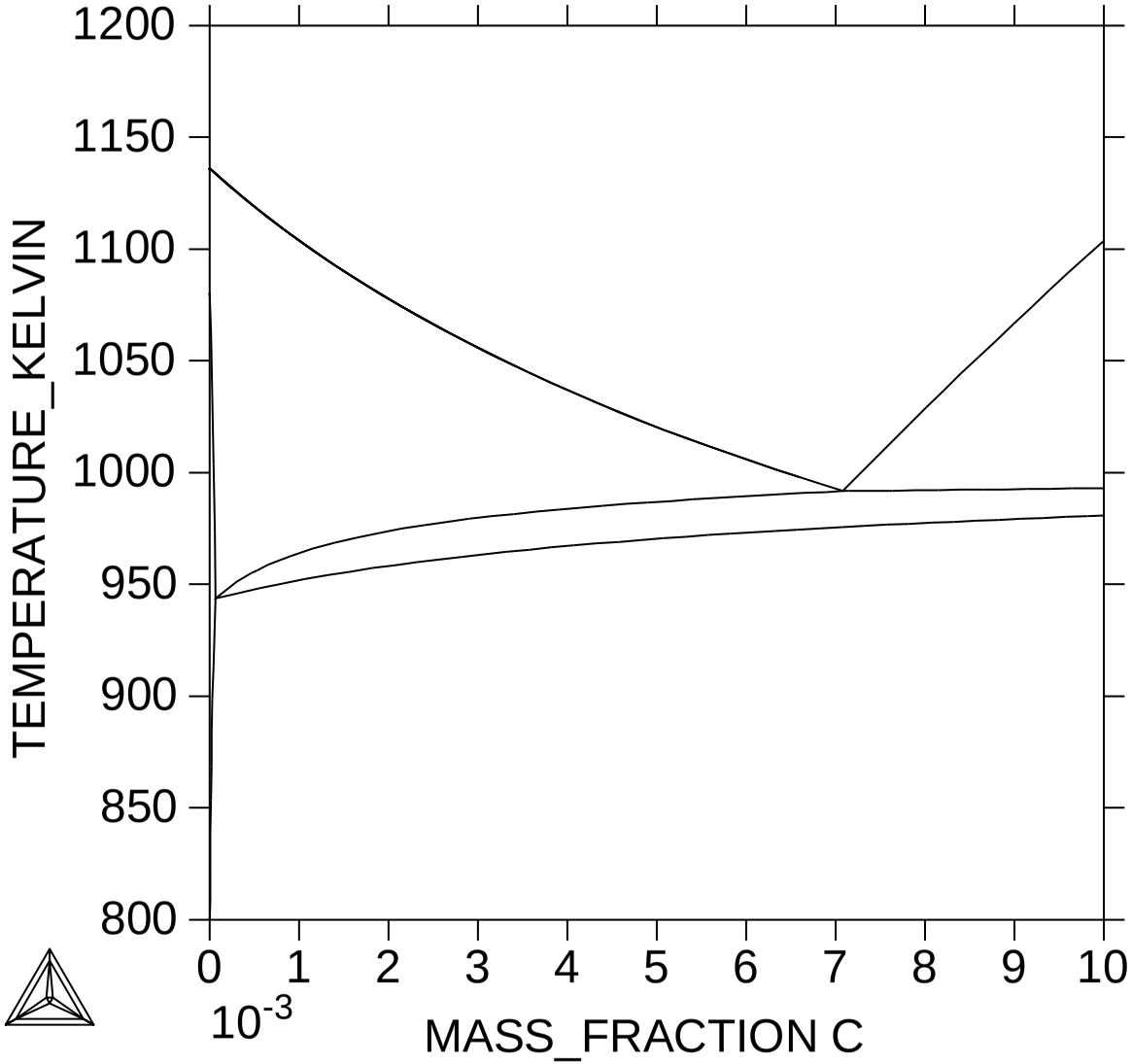
THERMO-CALC (2009.04.15:03.03) :example 23g
DATABASE:TCFE6
W(MN)=1.50451E-2, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.;



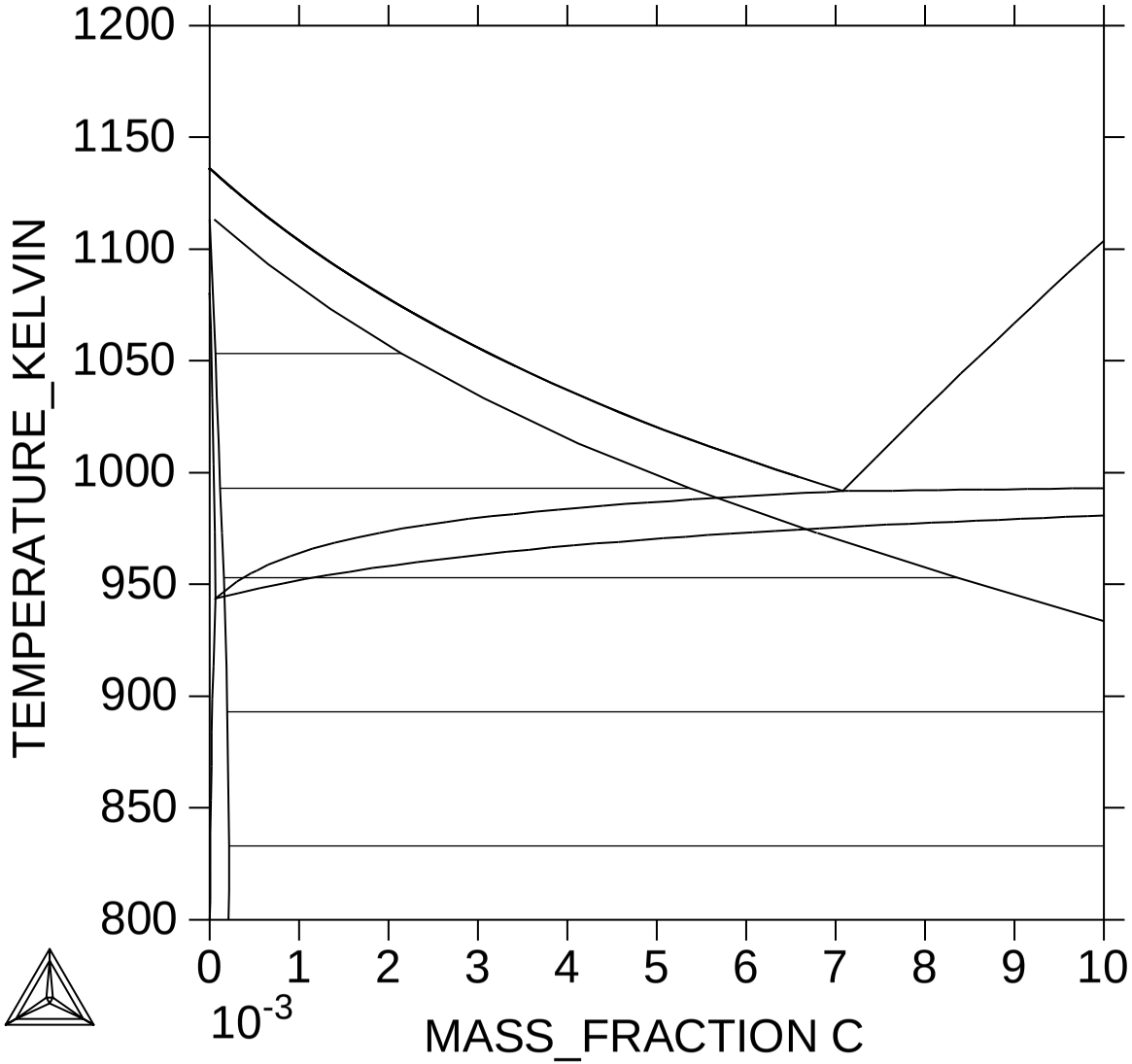
THERMO-CALC (2009.04.15:03.03) :example 23h
DATABASE:TCFE6
W(MN)=1.50451E-2, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.;



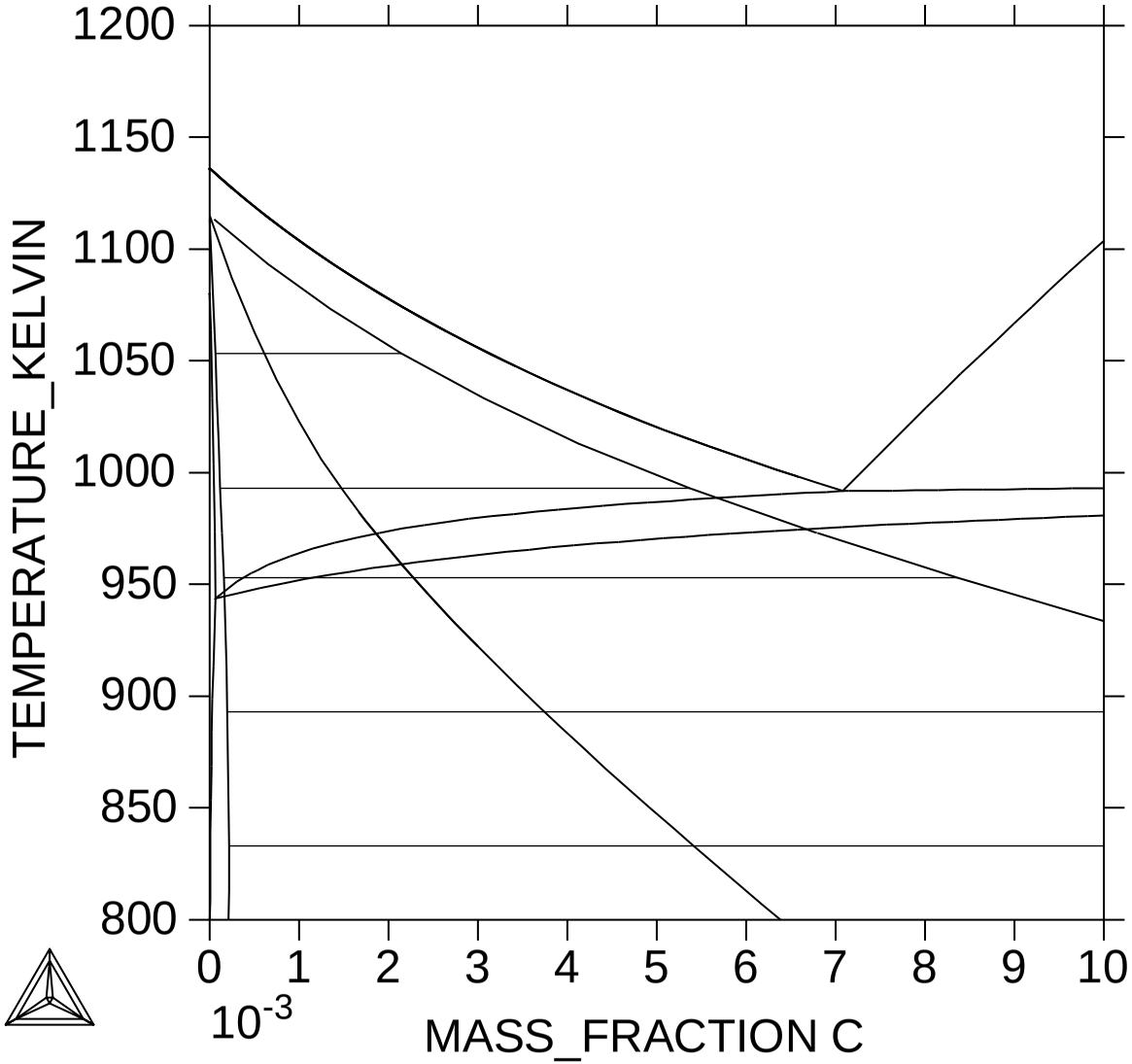
THERMO-CALC (2009.04.15:03.03) :example 23i
DATABASE:TCFE6
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1;

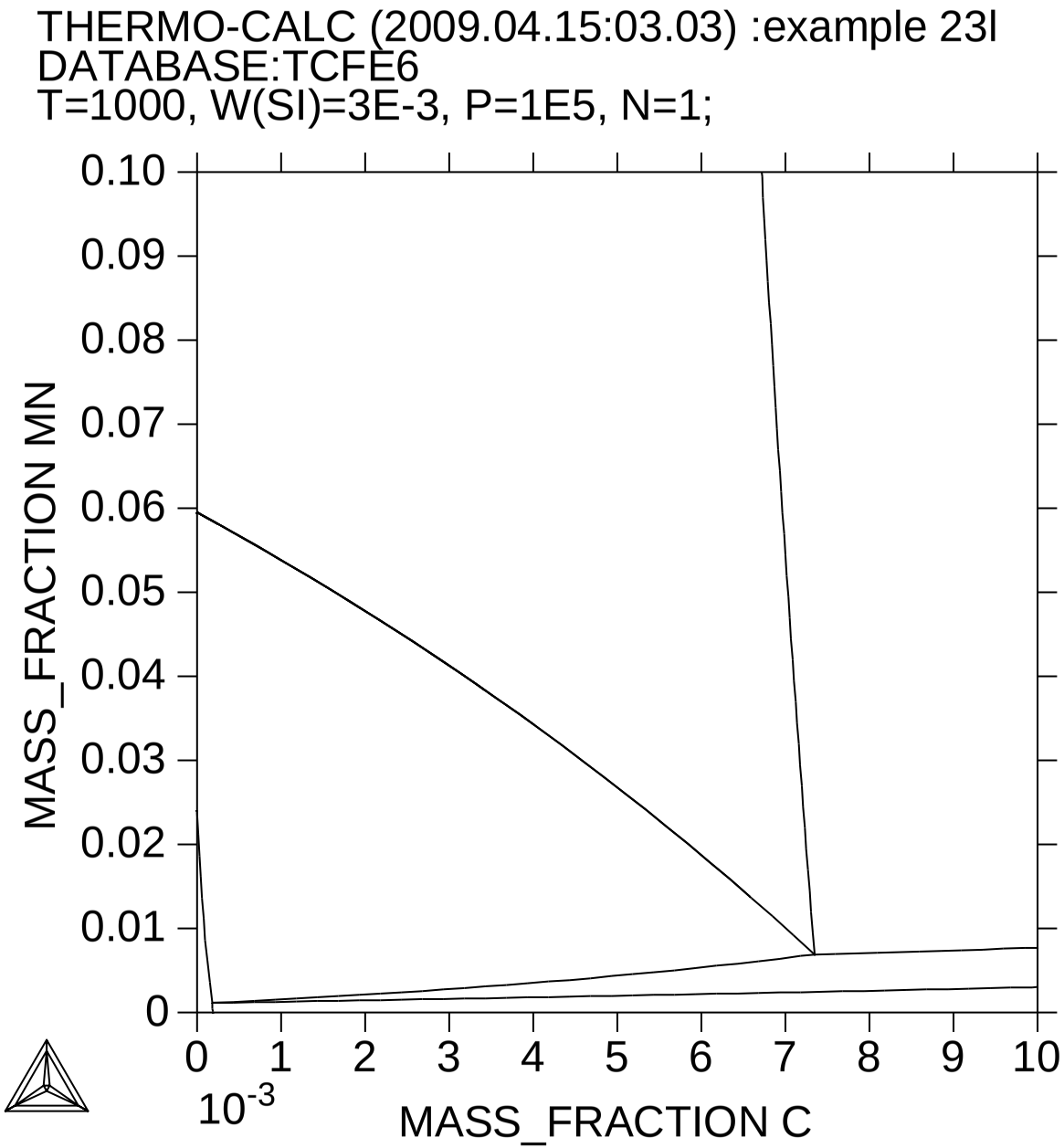


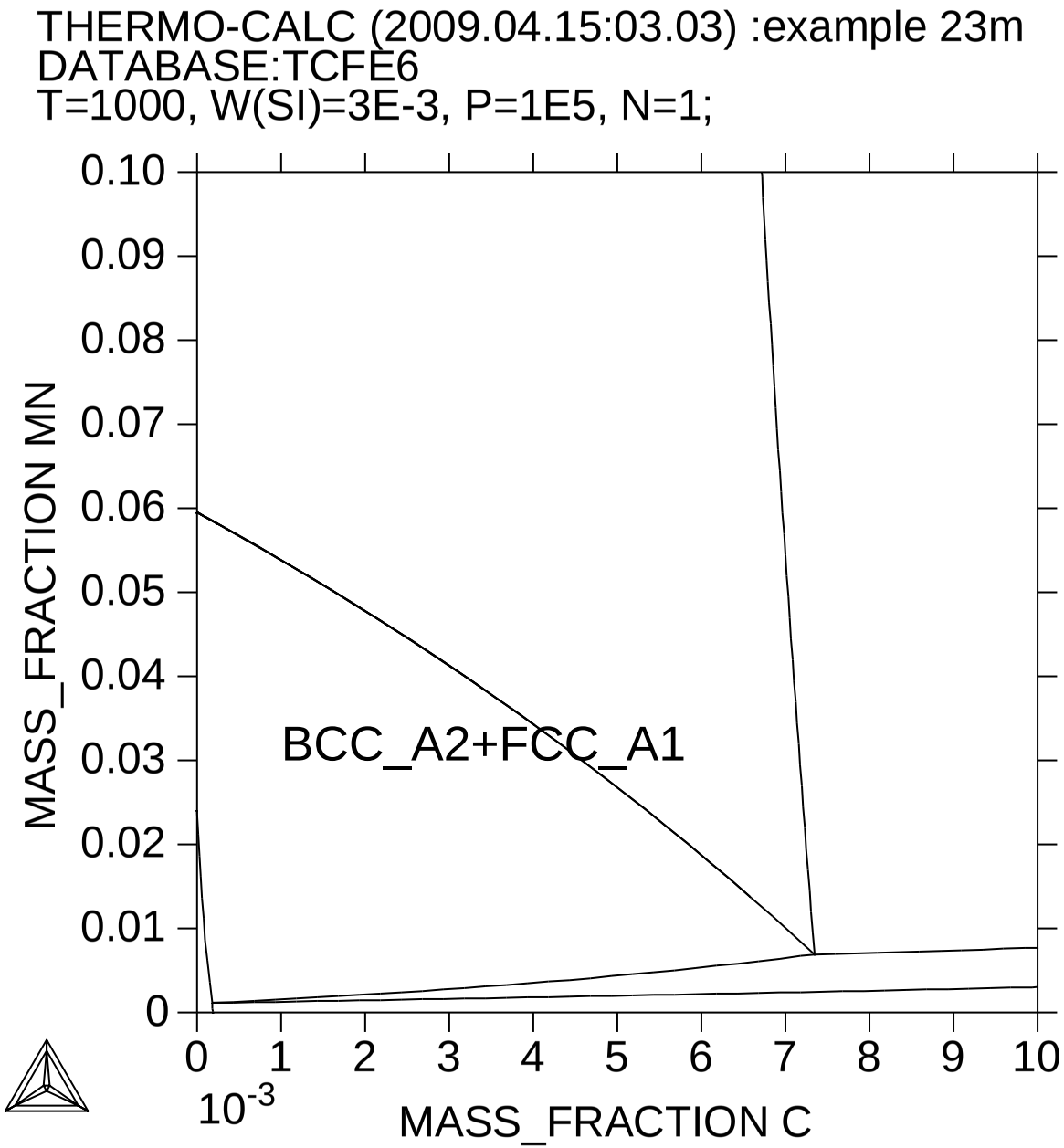
THERMO-CALC (2009.04.15:03.03) :example 23j
DATABASE:TCFE6
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1;



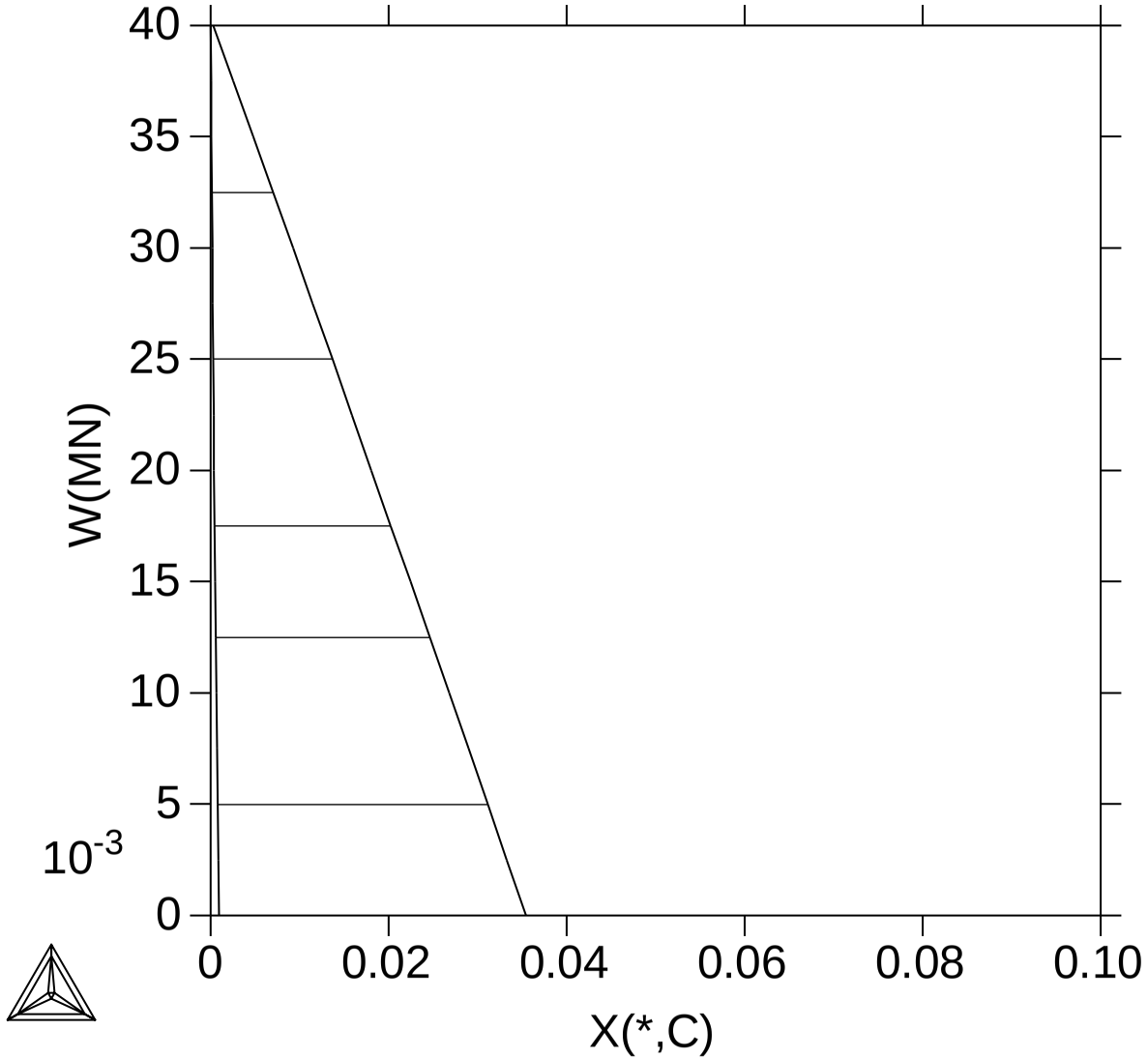
THERMO-CALC (2009.04.15:03.03) :example 23k
DATABASE:TCFE6
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1;



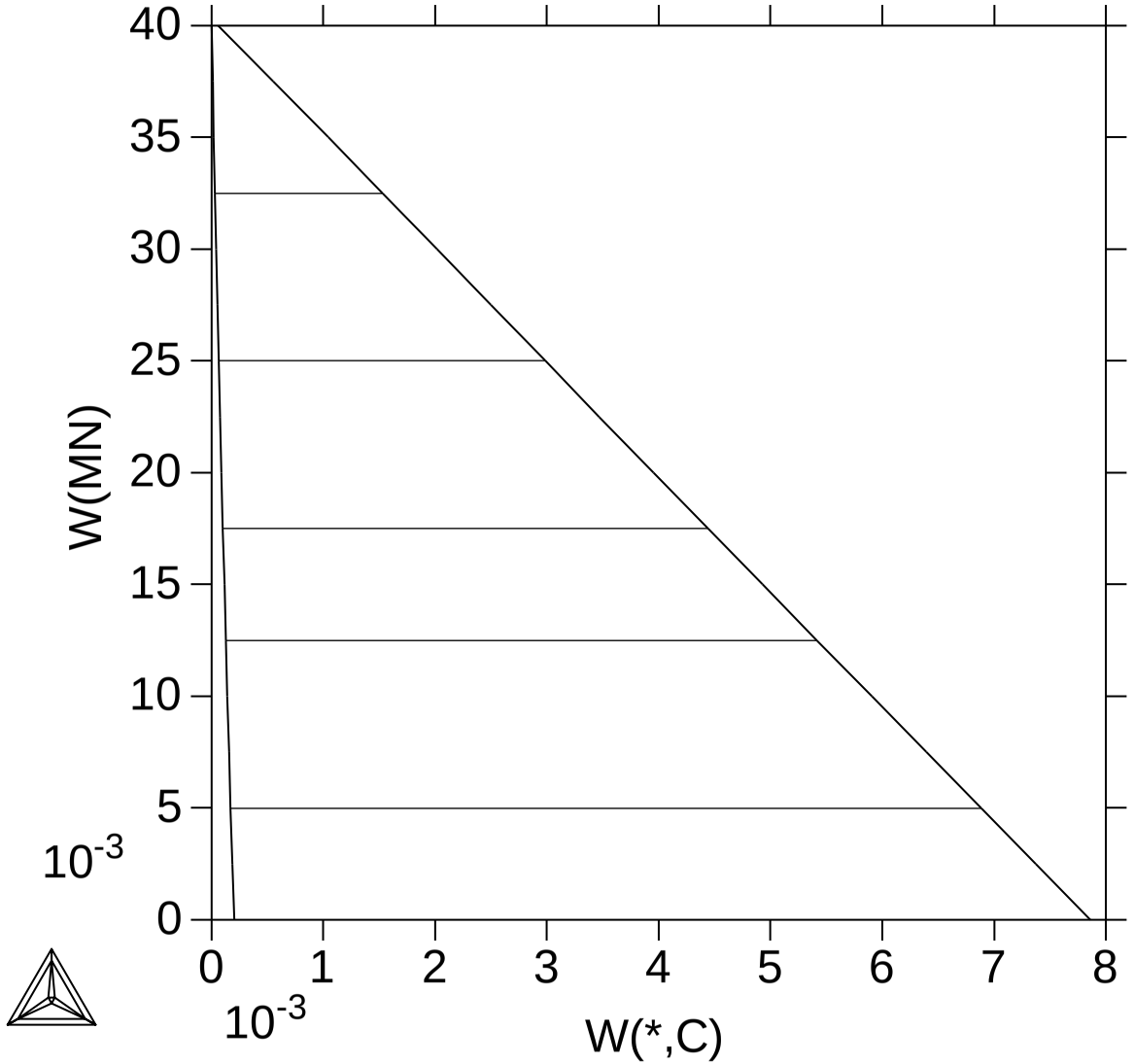

THERMO-CALC (2009.04.15:03.03) :example 23l
DATABASE:TCFE6
T=1000, W(SI)=3E-3, P=1E5, N=1;
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
MASS_FRACTION MN
0
1
2
3
4
5
6
7
8
9
10
10-3
MASS_FRACTION C

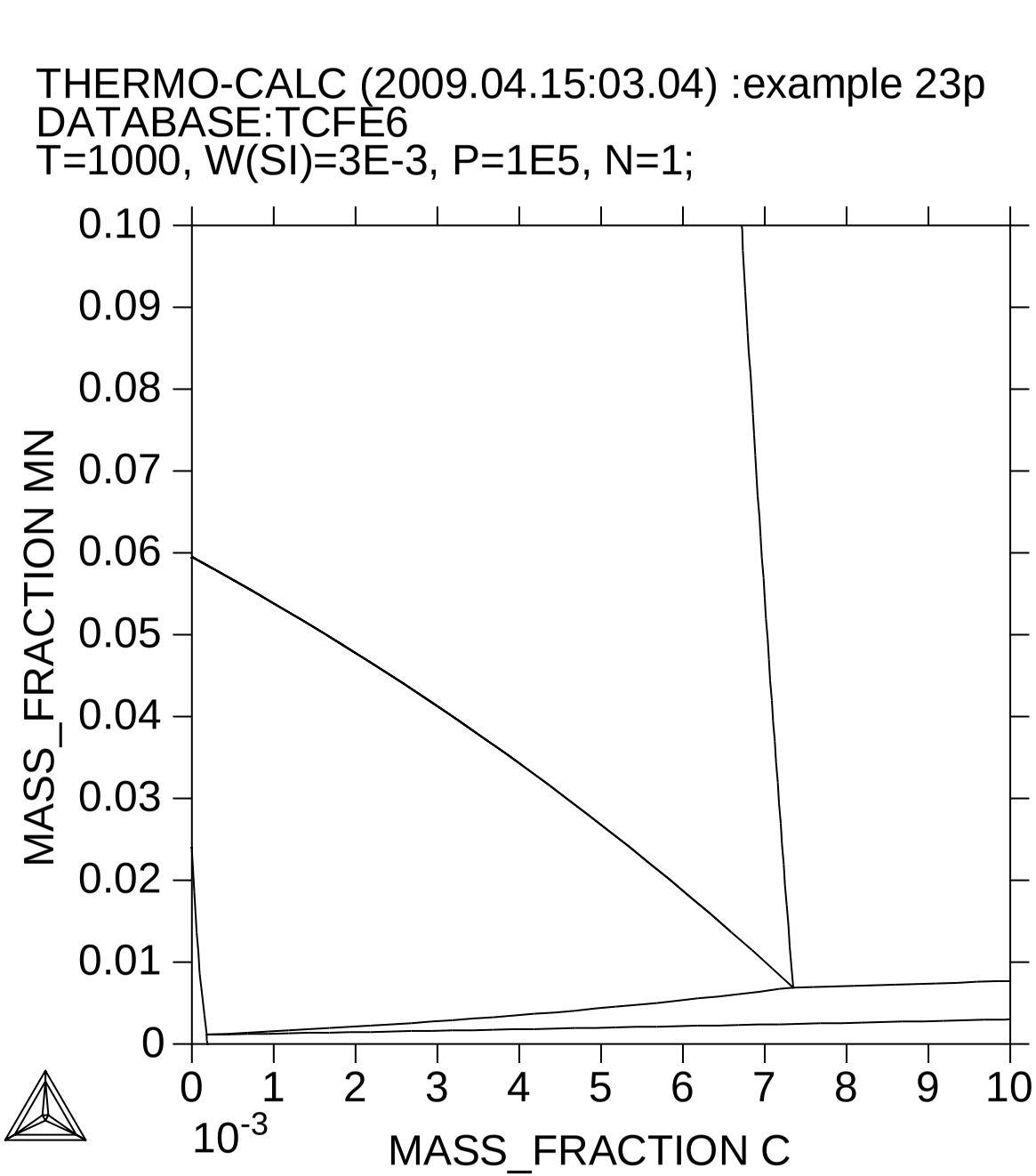

THERMO-CALC (2009.04.15:03.03) :example 23m
DATABASE:TCFE6
T=1000, W(SI)=3E-3, P=1E5, N=1;
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
MASS_FRACTION MN
BCC_A2+FCC_A1
0
1
2
3
4
5
6
7
8
9
10
10-3
MASS_FRACTION C

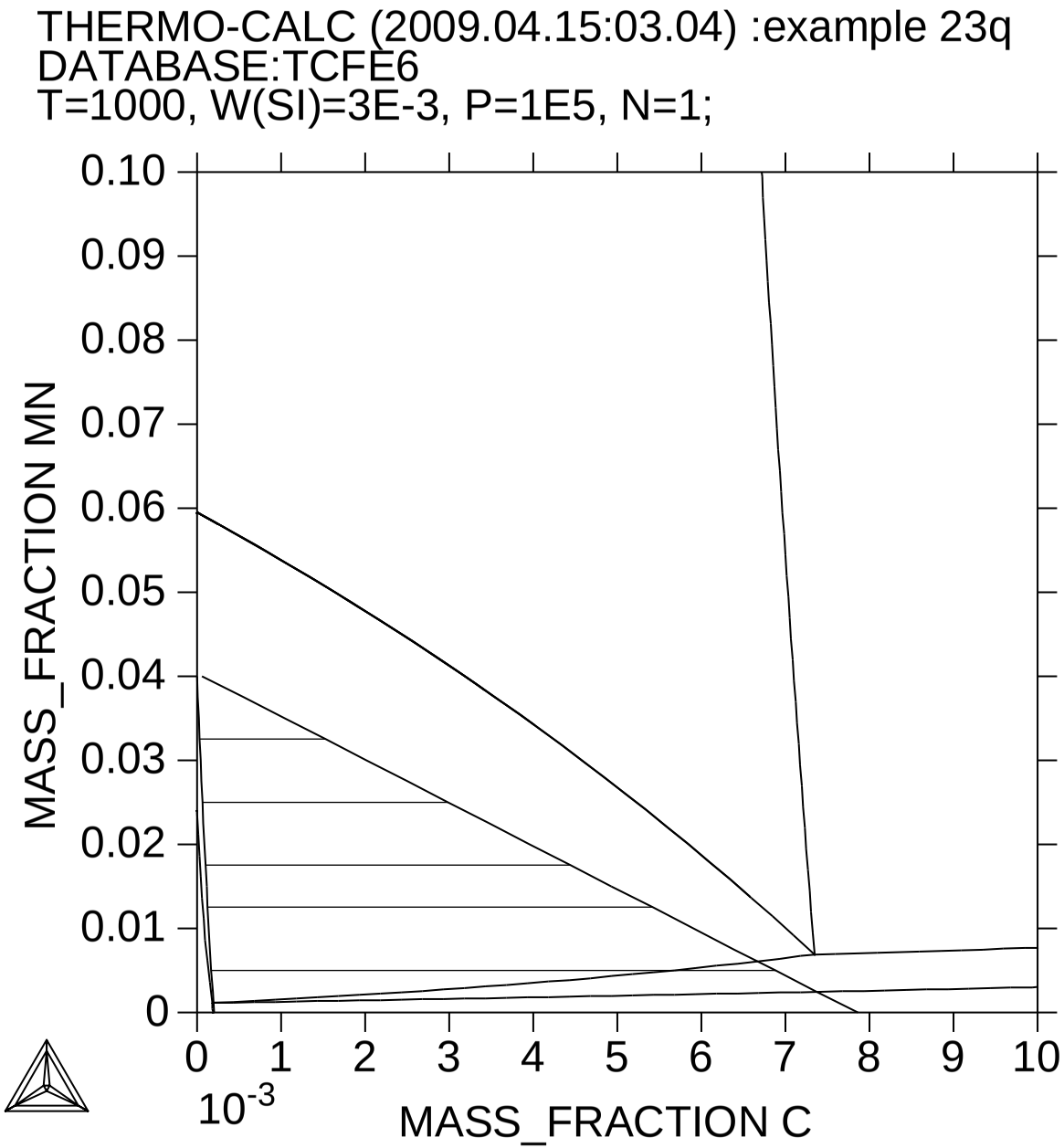
THERMO-CALC (2009.04.15:03.04) :example 23n
DATABASE:TCFE6
T=1000, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.;



THERMO-CALC (2009.04.15:03.04) :example 23o
DATABASE:TCFE6
T=1000, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.;




THERMO-CALC (2009.04.15:03.04) :example 23p
DATABASE:TCFE6
T=1000, W(SI)=3E-3, P=1E5, N=1;
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
MASS_FRACTION MN
0
1
2
3
4
5
6
7
8
9
10
10-3
MASS_FRACTION C


THERMO-CALC (2009.04.15:03.04) :example 23q
DATABASE:TCFE6
T=1000, W(SI)=3E-3, P=1E5, N=1;
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
MASS_FRACTION MN
0
1
2
3
4
5
6
7
8
9
10
10-3
MASS_FRACTION C

24

Simulation of the silicon arc furnace using the REACTOR module

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Use of the Thermo-Calc reactor for the silicon arc furnace
SYS: @@
SYS: @@ This is a very simple reactor model with output of gases at the top
SYS: @@ and output of condensed phases at the bottom. The gas phase from
SYS: @@ one segment will flow to higher segments, 80 % will react in the
SYS: @@ first above, 15% in the second above and 5 % in the third above.
SYS: @@ The condensed phases will flow downwards and all of it will go
SYS: @@ to the next lowest segment.
SYS: @@ Heat can be added at any module. The only way to specify the
SYS: @@ initial state of the reactants added to the reactor is to specify
SYS: @@ their heat content.
SYS: @@
SYS: @@ It is straightforward to add more facilities to this module and the
SYS: @@ source code to the reactor module is delivered with Thermo-Calc.
SYS: @@
SYS: @@ First fetch data
SYS: GO DAT
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: SW SSUB4
 Current database: SGTE Substances Database v4

 VA  DEFINED
TDB_SSUB4:
TDB_SSUB4: @@ Define-species means that data for just these species will be retrieved
TDB_SSUB4: @@ Define-system would mean that data for all combinations of the elements
TDB_SSUB4: @@ would be retrieved and this is not necessary here.
TDB_SSUB4: DEF-SPECIES C C1O1 C1O2 C1SI1 C2 C3 N1O1 N2 N4SI3
 C                       C1O1                    C1O2
 C1SI1                   C2                      C3
 N1O1                    N2                      N4SI3
   DEFINED
TDB_SSUB4: DEF-SP O O2 SI O1SI1 O2SI1
 O                       O2                      SI
 O1SI1                   O2SI1  DEFINED
TDB_SSUB4: GET
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
   C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      CARBON MONOXIDE <GAS>
      STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
   C1O2<G> T.C.R.A.S. Class: 2
      CARBON DIOXIDE <GAS>
   C1SI1<G> T.C.R.A.S. Class: 5
      SILICON CARBIDE <GAS>
                    :
                    :
                    :
   SI1 JANAF THERMOCHEMICAL TABLES SGTE **
      SILICON
      PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
      --U.D. 31/10/85
```

```
   O2SI1<TRIDYMITE> N.P.L.
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
 -OK-
TDB_SSUB4: GO G
 GIBBS ENERGY SYSTEM version  5.2
GES: CH-ST EL Y VA
 ELEMENT VA                      SUSPENDED
 SPECIES VA                      SUSPENDED
GES: L-ST
 GAS CONSTANT IN USER ENERGY UNITS:      8.31451000E+00
 1 BAR IN USER PRESSURE UNITS:           1.00000000E+05
 CURRENT VALUE OF TEMPERATURE (KELVIN):          298.15
 CURRENT VALUE OF PRESSURE (PASCAL):     1.00000000E+05

 CURRENT NUMBER OF ELEMENT     4

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00 E0000000
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00 E0000000
  1 C    GRAPHITE                  1.2011E+01  1.0540E+03  5.7400E+00 08000000
  2 N    1/2_MOLE_N2(GAS)          1.4007E+01  4.3350E+03  9.5751E+01 08000000
  3 O    1/2_MOLE_O2(GAS)          1.5999E+01  4.3410E+03  1.0252E+02 08000000
  4 SI   DIAMOND_A4                2.8085E+01  3.2175E+03  1.8820E+01 08000000

 CURRENT NUMBER OF PHASE      17

 PHASE                           STATUS   SUBLATTICES
   1 GAS                         88200000     1
   2 BETA_QUARTZ                 82200000     1
   3 C1SI1_ALPHA                 82200000     1
   4 C1SI1_BETA                  82200000     1
   5 CRISTOBALITE                82200000     1
   6 C_L                         82200000     1
   7 C_S                         82200000     1
   8 DIAMOND                     82200000     1
   9 LIQUID_SIO2                 82200000     1
  10 N4SI3_S                     82200000     1
  11 QUARTZ                      82200000     1
  12 QUARTZ_S2                   82200000     1
  13 SI_L                        82200000     1
  14 SI_S                        82200000     1
  15 TRIDYMITE                   82200000     1
  16 TRIDYMITE_S2                82200000     1
  17 TRIDYMITE_S3                82200000     1

 CURRENT NUMBER OF SPECIES    15

 SPECIES                                    STOICHIOMETRY
   1 C                           80800000   C
   2 C1O1                        00000000   C1O1
   3 C1O2                        00000000   C1O2
   4 C1SI1                       00000000   C1SI1
   5 C2                          00000000   C2
   6 C3                          00000000   C3
   7 N                           80800000   N
   8 N1O1                        00000000   N1O1
   9 N2                          00000000   N2
  10 N4SI3                       00000000   N4SI3
  11 O                           80800000   O
  12 O1SI1                       00000000   O1SI1
  13 O2                          00000000   O2
  14 O2SI1                       00000000   O2SI1
  15 SI                          80800000   SI
  16 VA                          D1800000   VA

GES: GO R
 Thermo-Calc REACTOR version 1.0 Feb 1992
REACTOR: ?
 AMEND_INPUT              CREATE_STAGE_BOXES       LIST_RECORDS
 AMEND_RECORD             EQUILIBRATE              MACRO-FILE-OPEN
 BACK                     EXECUTE_POLY3_COMMAND    READ_WORKSPACE
 CHANGE_SURROUNDINGS      EXIT                     SAVE_WORKSPACE
```

```
 CONTINUE_SIMULATION      GOTO_MODULE              SET_INTERACTIVE
 CREATE_DIVIDERS          HELP                     SHOW_PROBE
 CREATE_PIPES             INFORMATION              START_SIMULATION
 CREATE_PROBE             LIST_DESIGN
REACTOR: @@ Create a reactor with 4 segments which is heat controlled.
REACTOR: @@ At the top segment 1 mole of quartz (SiO2) and 1.8 mole of graphite (C)
REACTOR: @@ is added. A small amount of N is also added to simplify calculations.
REACTOR: @@ The reactants have room temperature.
REACTOR: @@ In the other three segments only heat is added.
REACTOR: @@
REACTOR: @@ A guess of the initial temperature in each segment must be provided.
REACTOR: @@
REACTOR: CREATE_STAGE
NUMBER OF STAGE BOXES /4/:  4
 YOU MUST FIRST DEFINE FEED FROM SURROUNDINGS!
GIVE FEED TO SYSTEM: N(C)=1.8
Input temperature /298.15/:
GIVE FEED TO SYSTEM: N(O2SI1)=1
Input temperature /298.15/:
GIVE FEED TO SYSTEM: H=876000
GIVE FEED TO SYSTEM: N(N2)=4e-4
Input temperature /298.15/:
GIVE FEED TO SYSTEM:

 GIVE FOR STAGE BOX     1
NAME: /SEGMENT_1/:
TYPE OF BOX /EQUILIBRIUM/:  EQUILIBRIUM
Is the stage heat controlled? /Y/:  Y
Initial guess of temperature? /1000/:  1750
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/:  gas
Phase name /REST/:  REST
 GIVE FOR STAGE BOX     2
NAME: /SEGMENT_2/:
TYPE OF BOX /EQUILIBRIUM/:  EQUILIBRIUM
Is the stage heat controlled? /Y/:  Y
Initial guess of temperature? /1000/:  1900
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/:  gas
Phase name /REST/:  REST
 GIVE FOR STAGE BOX     3
NAME: /SEGMENT_3/:
TYPE OF BOX /EQUILIBRIUM/:  EQUILIBRIUM
Is the stage heat controlled? /Y/:  Y
Initial guess of temperature? /1000/:  2050
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/:  gas
Phase name /REST/:  REST
 GIVE FOR STAGE BOX     4
NAME: /SEGMENT_4/:
TYPE OF BOX /EQUILIBRIUM/:  EQUILIBRIUM
Is the stage heat controlled? /Y/:  Y
Initial guess of temperature? /1000/:  2200
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/:  gas
Phase name /REST/:  REST
REACTOR: l-r
 Number:  0 name: SURROUNDINGS            stage box at:    23,
 Feed of C                       with  1.8000E+00 mol to record:    -1
 Feed of O2SI1                   with  1.0000E+00 mol to record:    -1
 Feed of heat  8.7600E+05 J to record:    -1
 Feed of N2                      with  4.0000E-04 mol to record:    -1

 Number:  1 name: SEGMENT_1               stage box at:    80, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:  2 name: SEGMENT_2               stage box at:   137, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1
```

```
 Number:  3 name: SEGMENT_3               stage box at:   194, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:  4 name: SEGMENT_4               stage box at:   251, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1
REACTOR: @@ Create dividers, one for distributing the gas from segment 2 to 4
REACTOR: @@ one for splitting the heat feed and one for splitting the feed on N2
REACTOR: create-div
Number of dividers /4/:  5
Number of outputs for divider 1: /3/:  2
Percent of input to output 1: /100/:  80
Number of outputs for divider 2: /3/:  3
Percent of input to output 1: /100/:  80 15
Number of outputs for divider 3: /3/:  3
Percent of input to output 1: /100/:  80 15
Number of outputs for divider 4: /3/:  3
Percent of input to output 1: /100/:  85 10
Number of outputs for divider 5: /3/:  4
Percent of input to output 1: /100/:  25 25 25
REACTOR: l-r
 Number:  0 name: SURROUNDINGS            stage box at:    23,
 Feed of C                        with  1.8000E+00 mol to record:    -1
 Feed of O2SI1                    with  1.0000E+00 mol to record:    -1
 Feed of heat  8.7600E+05 J to record:    -1
 Feed of N2                       with  4.0000E-04 mol to record:    -1

 Number:  1 name: SEGMENT_1               stage box at:    80, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:  2 name: SEGMENT_2               stage box at:   137, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:  3 name: SEGMENT_3               stage box at:   194, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:  4 name: SEGMENT_4               stage box at:   251, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:   5 name: DIVIDER_5               divider at:   308
   80 % of input to record:   -1
   20 % of input to record:   -1

 Number:   6 name: DIVIDER_6               divider at:   336
   80 % of input to record:   -1
   15 % of input to record:   -1
    5 % of input to record:   -1

 Number:   7 name: DIVIDER_7               divider at:   369
   80 % of input to record:   -1
   15 % of input to record:   -1
    5 % of input to record:   -1

 Number:   8 name: DIVIDER_8               divider at:   402
   85 % of input to record:   -1
   10 % of input to record:   -1
    5 % of input to record:   -1

 Number:   9 name: DIVIDER_9               divider at:   435
   25 % of input to record:   -1
   25 % of input to record:   -1
   25 % of input to record:   -1
   25 % of input to record:   -1
REACTOR: @@ Finally create the pipes between the segments first for the feed
REACTOR: c-pipe 0 1 1 8 9
 Feed of C
 Feed of O2SI1
 Feed of heat
```

```
 Input set to this divider
 Feed of N2
 Input set to this divider
 NO MORE OUTPUT RECORDS
REACTOR: @@ All solid phases are assumed to go down one segment
REACTOR: @@ The gas phase is assumed to go up, 80% to the next segment,
REACTOR: @@ 15% to the second next and 5% to the third segment above.
REACTOR: @@ output from stage boxes
REACTOR: c-pipe 1 0 2
 Output record for phase GAS
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 2 5 3
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 3 6 4
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 4 7 0
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: @@ output from dividers
REACTOR: c-pipe 5 1 0
 Output record for   80 % of input
 Output record for   20 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 6 2 1 0
 Output record for   80 % of input
 Output record for   15 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 7 3 2 1
 Output record for   80 % of input
 Output record for   15 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 8 4 3 2
 Output record for   85 % of input
 Output record for   10 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 9 1 2 3 4
 Output record for   25 % of input
 Output record for   25 % of input
 Output record for   25 % of input
 Output record for   25 % of input
 NO MORE OUTPUT RECORDS
REACTOR: l-r
 Number:  0 name: SURROUNDINGS            stage box at:    23,
 Feed of C                      with  1.8000E+00 mol to record:     1
 Feed of O2SI1                  with  1.0000E+00 mol to record:     1
 Feed of heat  8.7600E+05 J to record:     8
 Feed of N2                     with  4.0000E-04 mol to record:     9

 Number:  1 name: SEGMENT_1               stage box at:    80, H controlled
 Output for phase GAS                     to record:    0
 Output for phase REST                    to record:    2

 Number:  2 name: SEGMENT_2               stage box at:   137, H controlled
 Output for phase GAS                     to record:    5
 Output for phase REST                    to record:    3

 Number:  3 name: SEGMENT_3               stage box at:   194, H controlled
 Output for phase GAS                     to record:    6
 Output for phase REST                    to record:    4

 Number:  4 name: SEGMENT_4               stage box at:   251, H controlled
 Output for phase GAS                     to record:    7
```

```
 Output for phase REST                    to record:    0

 Number:   5 name: DIVIDER_5               divider at:   308
   80 % of input to record:    1
   20 % of input to record:    0

 Number:   6 name: DIVIDER_6               divider at:   336
   80 % of input to record:    2
   15 % of input to record:    1
    5 % of input to record:    0

 Number:   7 name: DIVIDER_7               divider at:   369
   80 % of input to record:    3
   15 % of input to record:    2
    5 % of input to record:    1

 Number:   8 name: DIVIDER_8               divider at:   402
   85 % of input to record:    4
   10 % of input to record:    3
    5 % of input to record:    2

 Number:   9 name: DIVIDER_9               divider at:   435
   25 % of input to record:    1
   25 % of input to record:    2
   25 % of input to record:    3
   25 % of input to record:    4
REACTOR: save tcex24 y
REACTOR: @@ Now start the process
REACTOR: read tcex24
REACTOR:
REACTOR: @@ The output for each iteration will consist of the conditions set in
REACTOR: @@ each segment, and the user may select some state variables also,
REACTOR: @@ in this case NP($) meaning moles of stable phases
REACTOR: @@ After each loop the temperatures in all segments are listed
REACTOR: @@
REACTOR: @@ We want to achive a reactor where only Si<L> leaves at the bottom.
REACTOR: START
Max number of loops: /10/:  50
Output file: /SCREEN/:
Output conditions? /Y/:
Output variables: /T BP($)/:  T BP($)
 >>> DATA AT ITERATION    1 FROM STAGE    1
 T=1750, P=1E5, N(C)=1.8, N(N)=2E-4, N(O)=2, N(SI)=1
 DEGREES OF FREEDOM 0
T= 1.750000E+03
 BP(GAS)=8.3899237E-3, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=3.9560635E-3, BP(CRISTOBALITE)=60.077021, BP(C_L)=0,
    BP(C_S)=21.616235, BP(DIAMOND)=0, BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0,
    BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    1 FROM STAGE    2
 T=1900, P=1E5, N(C)=1.7998, N(N)=2E-4, N(O)=1.9998, N(SI)=0.999999
 DEGREES OF FREEDOM 0
T= 1.900000E+03
 BP(GAS)=35.781375, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.515817, BP(CRISTOBALITE)=22.402821, BP(C_L)=0,
    BP(C_S)=0, BP(DIAMOND)=0, BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    1 FROM STAGE    3
 T=2050, P=1E5, N(C)=0.586488, N(N)=2E-4, N(O)=0.745729, N(SI)=0.959352
 DEGREES OF FREEDOM 0
T= 2.050000E+03
 BP(GAS)=1.1001909E-2, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.51327, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(LIQUID_SIO2)=22.396537, BP(N4SI3_S)=0, BP(QUARTZ)=0,
    BP(QUARTZ_S2)=0, BP(SI_L)=6.3106226E-4, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    1 FROM STAGE    4
 T=2200, P=1E5, N(C)=0.586424, N(N)=2E-4, N(O)=0.74552, N(SI)=0.959207
 DEGREES OF FREEDOM 0
T= 2.200000E+03
 BP(GAS)=27.369406, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=9.7781173, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
```

```
   BP(DIAMOND)=0, BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
   BP(QUARTZ_S2)=0, BP(SI_L)=8.7657156, BP(SI_S)=0, BP(TRIDYMITE)=0,
   BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    2 FROM STAGE    1
 H=-9.69232E5, P=1E5, N(C)=2.78779, N(N)=4E-4, N(O)=3.04056, N(SI)=1.0527
 DEGREES OF FREEDOM 0
T= 1.098651E+03
 BP(GAS)=25.395954, BP(BETA_QUARTZ)=63.249404, BP(C1SI1_ALPHA)=0,
   BP(C1SI1_BETA)=0, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=23.055463,
   BP(DIAMOND)=0, BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
   BP(QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
   BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    2 FROM STAGE    2
 H=-8.37416E5, P=1E5, N(C)=1.97096, N(N)=3.9E-4, N(O)=2.2174, N(SI)=1.1133
 DEGREES OF FREEDOM 0
T= 1.764644E+03
 BP(GAS)=2.577186E-2, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
   BP(C1SI1_BETA)=0.19891754, BP(CRISTOBALITE)=66.592185, BP(C_L)=0,
   BP(C_S)=23.605007, BP(DIAMOND)=0, BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0,
   BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
   BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    2 FROM STAGE    3
 H=-7.72457E5, P=1E5, N(C)=2.24429, N(N)=3.6E-4, N(O)=2.81309, N(SI)=1.43588
 DEGREES OF FREEDOM 0
T= 1.785830E+03
 BP(GAS)=28.121361, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
   BP(C1SI1_BETA)=21.054185, BP(CRISTOBALITE)=54.435284, BP(C_L)=0,
   BP(C_S)=8.6836045, BP(DIAMOND)=0, BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0,
   BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
   BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    2 FROM STAGE    4
 H=33660.3, P=1E5, N(C)=1.24807, N(N)=2E-4, N(O)=1.812, N(SI)=1.4311
 DEGREES OF FREEDOM 0
T= 2.447572E+03
 BP(GAS)=60.210328, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
   BP(C1SI1_BETA)=0.5584813, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
   BP(DIAMOND)=0, BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
   BP(QUARTZ_S2)=0, BP(SI_L)=23.407066, BP(SI_S)=0, BP(TRIDYMITE)=0,
   BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 ================================
                           :
                           :
                           :

 >>> DATA AT ITERATION   50 FROM STAGE    1
 H=-9.91627E5, P=1E5, N(C)=2.84556, N(N)=6.784E-4, N(O)=3.8154, N(SI)=1.76988
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475748, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
   BP(C1SI1_BETA)=25.204308, BP(CRISTOBALITE)=68.127483, BP(C_L)=0,
   BP(C_S)=8.1297561, BP(DIAMOND)=0, BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0,
   BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
   BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   50 FROM STAGE    2
 H=-9.24205E5, P=1E5, N(C)=2.0559, N(N)=5.18E-4, N(O)=4.00492, N(SI)=2.7494
 DEGREES OF FREEDOM 0
T= 2.062992E+03
 BP(GAS)=61.98157, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
   BP(C1SI1_BETA)=38.054155, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
   BP(DIAMOND)=0, BP(LIQUID_SIO2)=65.956461, BP(N4SI3_S)=0, BP(QUARTZ)=0,
   BP(QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
   BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   50 FROM STAGE    3
 H=-8.11307E5, P=1E5, N(C)=1.65476, N(N)=3.6E-4, N(O)=3.73665, N(SI)=2.88298
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.390078, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
   BP(C1SI1_BETA)=35.36872, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
   BP(DIAMOND)=0, BP(LIQUID_SIO2)=57.872886, BP(N4SI3_S)=0, BP(QUARTZ)=0,
   BP(QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
   BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   50 FROM STAGE    4
 H=9243.41, P=1E5, N(C)=0.882101, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84532
```

```
 DEGREES OF FREEDOM 0
T= 2.223483E+03
 BP(GAS)=70.772932, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0, BP(DIAMOND)=0,
    BP(LIQUID_SIO2)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
    BP(SI_L)=22.471475, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
REACTOR: @@ Currently no nice output is provided in this module. Use POLY-3
REACTOR: @@ to list the constitution in each segment
REACTOR: GO P-3
POLY_3: L-E
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =  1004, label A0  , database: SSUB4

 Conditions:
 H=9243.41, P=1E5, N(C)=0.882101, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84532
 DEGREES OF FREEDOM 0

 Temperature   2223.48 K (  1950.33 C),  Pressure  1.000000E+05
 Number of moles of components  4.65405E+00,  Mass in grams  9.32444E+01
 Total Gibbs energy -1.35902E+06,  Enthalpy  9.24341E+03,  Volume  3.56321E-01

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       8.8210E-01  1.1363E-01 5.0909E-03 -9.7618E+04 SER
 N                       2.0000E-04  3.0044E-05 8.4815E-09 -3.4359E+05 SER
 O                       1.9264E+00  3.3054E-01 1.4658E-13 -5.4632E+05 SER
 SI                      1.8453E+00  5.5581E-01 1.5640E-03 -1.1944E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 3.8539E+00, Mass 7.0773E+01, Volume fraction 1.0000E+00  Mass fractions:
 O   4.35491E-01  SI  4.14767E-01  C   1.49703E-01  N   3.95829E-05
 Constitution:
 O1SI1  5.41812E-01  C1O2   2.03425E-05  C      2.35251E-10  O2     9.77965E-14
 C1O1   4.57645E-01  O2SI1  1.70445E-06  N1O1   7.37233E-11
 SI     4.69565E-04  C1SI1  3.44130E-09  C3     4.10868E-12
 N2     5.18835E-05  O      9.79916E-10  C2     3.46768E-12

 SI_L                         Status ENTERED     Driving force  0.0000E+00
 Moles 8.0012E-01, Mass 2.2471E+01, Volume fraction 0.0000E+00  Mass fractions:
 SI  1.00000E+00  C   0.00000E+00  O   0.00000E+00  N   0.00000E+00
POLY_3: @@ This equilibrium is valid for the fourth segment. Note it is
POLY_3: @@ identified with number 1004. The other have numbers 1001, 1002 and 1003.
POLY_3: @@ Good luck for future work with this!
POLY_3: go sys
SYS: set-inter
SYS:SYS: CPU time           2  seconds
```

25

Simulation of steel refining

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@ Raw iron used to produce steel usually has very high carbon and
SYS: @@ silicon content. Oxygen is thus blown into the furnace to burn off
SYS: @@ carbon. Lime (CaO) is added to form a slag with silica, and the slag
SYS: @@ can be removed. Alloying elements, such as Mn, Ni, Cr and V are added
SYS: @@ to produce desired steel. Since the reaction between oxygen and
SYS: @@ carbon will increase the temperature, scrap iron is added in order to
SYS: @@ keep the temperature constant (we assume the furnace is isolated
SYS: @@ and no heat is lost to the environment). This is a typical steel
SYS: @@ refining process.
SYS: @@
SYS: @@ This example simulates blowing oxygen into a liquid steel of one
SYS: @@ metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles
SYS: @@ of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant
SYS: @@ is the way to simulate the isolation of the furnace. The oxygen
SYS: @@ will react with carbon and increase the temperature. After blowing
SYS: @@ a certain amount of oxygen, scrap iron is added to keep the temperature
SYS: @@ constant.
SYS: @@
SYS: set-log ex25,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: @@ In this example we use data from the slag database
TDB_TCFE6: sw slag2
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Fe-containing Slag Database v2

 FE                      O  DEFINED
TDB_SLAG2: d-sys ca si mn c
   ... the command in full is DEFINE_SYSTEM
 CA                      SI                      MN
 C  DEFINED
TDB_SLAG2: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 GAS:G       :C C2 C3 C4 C5 C60 C1O1 C1O2 C2O1 C3O2 C1SI1 C1SI2 C2SI1
  C5FE1O5 CA CA2 CA1O1 FE FE2 FE1O1 FE1O2 MN MN1O1 MN1O2 O O2 O3 O1SI1 O2SI1
  O2SI2 SI SI2 SI3:
  > The gaseous mixture is handled by the ideal gas model.
 FE_LIQUID:L :C CA FE MN O SI:
  > Fe-rich liquid mixture handled by Sigworth-Elliot-Hillert Model.
 SLAG:L      :A0_01_C00C04_12_SIO2 A0_01_C00C10_23_FE2O3 A0_01_C00C16_11_FEO
  A0_01_C00C22_11_MNO A0_01_C00C27_11_CAO A0_01_C04C10_SIFE
  A0_01_C04C16_SIFE A0_01_C04C22_SIMN A0_01_C04C27_SICA A0_01_C10C16_FEFE
  A0_01_C10C22_FEMN A0_01_C10C27_FECA A0_01_C16C22_FEMN A0_01_C16C27_FECA
  A0_01_C22C27_MNCA:
  > Slag phase handled by Kapoor-Frohberg-Gaye Quasichemical Cell Model.
 FEOLIQ      :FEO:
  > Pure FeO liquid phase.
 SIO2        :SIO2:
 FE2O3       :FE2O3:
 WUSTITE     :FEO:
 MNO         :MNO:
 CAO         :CAO:
 CAO_SIO2    :CAO:SIO2:
 CA3O3_SI2O4 :CAO:SIO2:
 CA2O2_SIO2  :CAO:SIO2:
 CA3O3_SIO2  :CAO:SIO2:
 FE2O2_SIO2  :FEO:SIO2:
 MNO_SIO2    :MNO:SIO2:
```

```
 MN2O2_SIO2  :MNO:SIO2:
 GRAPHITE    :C:
TDB_SLAG2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'SLAG2 (2006): TCS Fe-Containing Slag Database, V2.2, owned and provided
      by Thermo-Calc Software.'
  'TCMP2 (2004): TCS Materials Processing Database, V2.3, owned and provided
      by Thermo-Calc Software.'
 -OK-
TDB_SLAG2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ Assume we have one ton (1e6 gram) liquid steel with a composition
POLY_3: @@ set of 4 w/o C, 2 w/o Si and 1 w/o Mn.
POLY_3: s-c t=1673,p=1e5,b(fe)=1e6,w(c)=.04,w(si)=.02,w(mn)=.01
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2
 DEGREES OF FREEDOM 2
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ To remove Si, add a small amount of top slag consisting of
POLY_3: @@ pure lime (CaO), 5.6 kg equivalent to 100 moles of CaO
POLY_3: s-i-a n(cao)=100
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
    N(O)=100
 DEGREES OF FREEDOM 0
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Prior to version R, in some cases one needs to use SET_ALL_START_VALUES to
POLY_3: @@ calculate stable equilibria. In version R, the Global Minimization
POLY_3: @@ procedure will automatically find the global minimum in Gibbs energy space.
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         2114  grid points in            1  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       3 s, total time     4  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG2

 Conditions:
 T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
    N(O)=100
 DEGREES OF FREEDOM 0

 Temperature   1673.00 K (  1399.85 C),  Pressure  1.000000E+05
 Number of moles of components  2.26739E+04,  Mass in grams  1.08130E+06
 Total Gibbs energy -2.19006E+09,  Enthalpy  1.32046E+09,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.6010E+03  4.0000E-02 7.5454E-02 -3.5947E+04 SER
 CA                      1.0000E+02  3.7065E-03 1.4244E-08 -2.5131E+05 SER
 FE                      1.7906E+04  9.2481E-01 7.1047E-04 -1.0084E+05 SER
 MN                      1.9682E+02  1.0000E-02 5.1231E-06 -1.6945E+05 SER
 O                       1.0000E+02  1.4796E-03 6.6380E-17 -5.1817E+05 SER
 SI                      7.7002E+02  2.0000E-02 1.3697E-06 -1.8780E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
```

```
 Moles 2.2474E+04, Mass 1.0757E+06, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.29634E-01  SI  2.01042E-02  CA  6.94868E-07
 C   4.02085E-02  MN  1.00521E-02  O   2.36693E-07

 CAO                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.9995E+02, Mass 5.6064E+03, Volume fraction 0.0000E+00  Mass fractions:
 CA  7.14696E-01  C   0.00000E+00  FE  0.00000E+00
 O   2.85304E-01  MN  0.00000E+00  SI  0.00000E+00

 CA3O3_SIO2                 Status ENTERED     Driving force  0.0000E+00
 Moles 1.2313E-02, Mass 3.1236E-01, Volume fraction 0.0000E+00  Mass fractions:
 CA  5.26617E-01  SI  1.23010E-01  FE  0.00000E+00
 O   3.50373E-01  C   0.00000E+00  MN  0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 CAO                    ENTERED    0.00000000E+00  1.99954496E+02
 CA3O3_SIO2             ENTERED    0.00000000E+00  1.23129805E-02
 FE_LIQUID              ENTERED    0.00000000E+00  2.24739656E+04
 CA2O2_SIO2             ENTERED   -1.47428604E-01  0.00000000E+00
 GRAPHITE               ENTERED   -1.87047122E-01  0.00000000E+00
 SLAG                   ENTERED   -3.28308988E-01  0.00000000E+00
 CA3O3_SI2O4            ENTERED   -4.94210601E-01  0.00000000E+00
 CAO_SIO2               ENTERED   -1.01925287E+00  0.00000000E+00
 GAS                    ENTERED   -2.40053972E+00  0.00000000E+00
 SIO2                   ENTERED   -3.67977814E+00  0.00000000E+00
 MNO_SIO2               ENTERED   -3.69974441E+00  0.00000000E+00
 MN2O2_SIO2             ENTERED   -3.77258386E+00  0.00000000E+00
 MNO                    ENTERED   -4.56640807E+00  0.00000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.81642570E+00
 FE2O2_SIO2 FEOLIQ WUSTITE FE2O3
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ The steel bath will be insulated so no heat disappears
POLY_3: @@ while blowing oxygen. This means that the enthalpy of the
POLY_3: @@ system is constant and the temperature may increase. Set these
POLY_3: @@ conditions
POLY_3: s-c h
   ... the command in full is SET_CONDITION
Value /1.32045762E+09/:
POLY_3: s-c t=none
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=100,
    H=1.32046E9
 DEGREES OF FREEDOM 0
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ When we calculate now we should get exactly the same temperature
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         2114  grid points in           0  s
     6 ITS,  CPU TIME USED   3 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1673.
POLY_3: @@ Voila! The same equilibrium calculated with different conditions
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG2

 Conditions:
 P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=100,
    H=1.32046E9
 DEGREES OF FREEDOM 0

 Temperature   1673.00 K (  1399.85 C),  Pressure  1.000000E+05
 Number of moles of components  2.26739E+04,  Mass in grams  1.08130E+06
 Total Gibbs energy -2.19006E+09,  Enthalpy  1.32046E+09,  Volume  0.00000E+00
```

```
 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.6010E+03  4.0000E-02 7.5454E-02 -3.5947E+04 SER
 CA                      1.0000E+02  3.7065E-03 1.4244E-08 -2.5131E+05 SER
 FE                      1.7906E+04  9.2481E-01 7.1047E-04 -1.0084E+05 SER
 MN                      1.9682E+02  1.0000E-02 5.1231E-06 -1.6945E+05 SER
 O                       1.0000E+02  1.4796E-03 6.6380E-17 -5.1817E+05 SER
 SI                      7.7002E+02  2.0000E-02 1.3697E-06 -1.8780E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.2474E+04, Mass 1.0757E+06, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.29634E-01  SI  2.01042E-02  CA  6.94868E-07
 C   4.02085E-02  MN  1.00521E-02  O   2.36693E-07

 CAO                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.9995E+02, Mass 5.6064E+03, Volume fraction 0.0000E+00  Mass fractions:
 CA  7.14696E-01  C   0.00000E+00  FE  0.00000E+00
 O   2.85304E-01  MN  0.00000E+00  SI  0.00000E+00

 CA3O3_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 1.2313E-02, Mass 3.1236E-01, Volume fraction 0.0000E+00  Mass fractions:
 CA  5.26617E-01  SI  1.23010E-01  FE  0.00000E+00
 O   3.50373E-01  C   0.00000E+00  MN  0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Now set the oxygen content as independent variable
POLY_3: @@ and blow up to 2000 moles of O (i.e. 1000 moles of O2 i.e. 22.4 m3)
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: n(o)
Min value /0/:  100
Max value /1/:  2000
Increment /47.5/:  100
POLY_3: save tcex25 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    100.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    100.000     for:
     FE_LIQUID
     CA3O3_SIO2
     CAO
 Global check of removing phase at  1.66663E+02
 Calculated     3 equilibria

 Phase Region from    166.663     for:
     FE_LIQUID
     CA3O3_SIO2
 Global check of adding phase at  1.66799E+02
 Calculated     3 equilibria

 Phase Region from    166.799     for:
     FE_LIQUID
     CA2O2_SIO2
     CA3O3_SIO2
 Global check of removing phase at  2.00157E+02
 Calculated     4 equilibria

 Phase Region from    200.157     for:
     FE_LIQUID
     CA2O2_SIO2
 Global check of adding phase at  2.02166E+02
 Calculated     3 equilibria

 Phase Region from    202.166     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  1.00000E+03 .... OK
```

```
 Global test at  2.00000E+03 .... OK
 Terminating at    2000.00
 Calculated    21 equilibria
 *** Buffer saved on file: tcex25.POLY3
POLY_3: @@ Sometimes trouble here, error 1614 means all conditions not fullfilled.
POLY_3: @@ Try to start with more oxygen ...
POLY_3: read tcex25
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c n(o)
   ... the command in full is SET_CONDITION
Value /100/:  200
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         2114  grid points in           0  s
    94 ITS,  CPU TIME USED   3 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG2

 Conditions:
 P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=200,
    H=1.32046E9
 DEGREES OF FREEDOM 0

 Temperature   1723.42 K (  1450.27 C),  Pressure  1.000000E+05
 Number of moles of components  2.27812E+04,  Mass in grams  1.08302E+06
 Total Gibbs energy -2.34831E+09,  Enthalpy  1.32046E+09,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.6068E+03  4.0000E-02 6.5488E-02 -3.9060E+04 SER
 CA                      1.0000E+02  3.7006E-03 1.5356E-09 -2.9081E+05 SER
 FE                      1.7906E+04  9.2334E-01 6.2289E-04 -1.0577E+05 SER
 MN                      1.9713E+02  1.0000E-02 4.3101E-06 -1.7703E+05 SER
 O                       2.0000E+02  2.9545E-03 7.6249E-16 -4.9881E+05 SER
 SI                      7.7124E+02  2.0000E-02 1.2968E-06 -1.9424E+05 SER

 FE_LIQUID                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.2431E+04, Mass 1.0744E+06, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.30742E-01  SI  1.88553E-02  O   2.34486E-06
 C   4.03204E-02  MN  1.00801E-02  CA  1.80134E-08

 CA2O2_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 3.4836E+02, Mass 8.5714E+03, Volume fraction 0.0000E+00  Mass fractions:
 CA  4.65382E-01  SI  1.63060E-01  FE  0.00000E+00
 O   3.71558E-01  C   0.00000E+00  MN  0.00000E+00

 CA3O3_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 1.4085E+00, Mass 3.5732E+01, Volume fraction 0.0000E+00  Mass fractions:
 CA  5.26617E-01  SI  1.23010E-01  FE  0.00000E+00
 O   3.50373E-01  C   0.00000E+00  MN  0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ if still trouble, add that gas should be stable (gas dissolves all)
POLY_3: @@ by increasing oxygen content
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 CA3O3_SIO2              ENTERED    0.00000000E+00  1.40852525E+00
 CA2O2_SIO2              ENTERED    0.00000000E+00  3.48355040E+02
 FE_LIQUID               ENTERED    0.00000000E+00  2.24314368E+04
 SLAG                    ENTERED   -1.46657534E-01  0.00000000E+00
 CA3O3_SI2O4             ENTERED   -2.50033970E-01  0.00000000E+00
 GRAPHITE                ENTERED   -2.69878146E-01  0.00000000E+00
 CAO                     ENTERED   -4.78819867E-01  0.00000000E+00
 CAO_SIO2                ENTERED   -6.20216074E-01  0.00000000E+00
 GAS                     ENTERED   -1.30777329E+00  0.00000000E+00
 SIO2                    ENTERED   -2.64147120E+00  0.00000000E+00
 MNO_SIO2                ENTERED   -2.76455450E+00  0.00000000E+00
 MN2O2_SIO2              ENTERED   -2.88391269E+00  0.00000000E+00
 MNO                     ENTERED   -3.75773352E+00  0.00000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN -3.84036617E+00
```

```
 FE2O2_SIO2 FEOLIQ WUSTITE FE2O3
POLY_3: c-st p gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:  1
POLY_3: s-c n(o)=300
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         2114  grid points in           1  s
    37 ITS,  CPU TIME USED   4 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG2

 Conditions:
 P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=300,
    H=1.32046E9
 DEGREES OF FREEDOM 0

 Temperature   1737.41 K (  1464.26 C),  Pressure  1.000000E+05
 Number of moles of components  2.28885E+04,  Mass in grams  1.08474E+06
 Total Gibbs energy -2.42505E+09,  Enthalpy  1.32046E+09,  Volume  1.41396E+01

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.6125E+03  4.0000E-02 5.9862E-02 -4.0675E+04 SER
 CA                      1.0000E+02  3.6947E-03 1.1359E-11 -3.6405E+05 SER
 FE                      1.7906E+04  9.2188E-01 6.0707E-04 -1.0700E+05 SER
 MN                      1.9745E+02  1.0000E-02 4.1965E-06 -1.7886E+05 SER
 O                       3.0000E+02  4.4248E-03 1.1809E-14 -4.6327E+05 SER
 SI                      7.7247E+02  2.0000E-02 1.2680E-06 -1.9614E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 1.9576E+02, Mass 2.7425E+03, Volume fraction 1.0000E+00  Mass fractions:
 O   5.71009E-01  MN  3.26864E-04  FE  1.77084E-05
 C   4.28581E-01  SI  6.50792E-05  CA  9.33307E-08
 Constitution:
 C1O1     9.99604E-01  C2O1     3.60024E-11  O2       2.65004E-16
 MN       1.66700E-04  FE1O1    2.16563E-11  C1SI1    1.89897E-16
 C1O2     1.55481E-04  C2SI1    1.24191E-12  FE1O2    1.35522E-17
 O1SI1    6.49233E-05  O        1.07250E-12  CA2      4.52820E-18
 FE       8.88424E-06  CA1O1    1.56195E-13  MN1O2    4.07663E-18
 CA       6.52467E-08  FE2      1.23188E-13  C5       7.36602E-20
 O2SI2    4.12168E-10  C1SI2    3.31148E-14  SI3      6.62708E-20
 O2SI1    2.76336E-10  C        3.19274E-14  C4       3.28485E-20
 SI       2.45777E-10  C3       5.66532E-15  C5FE1O5  8.43862E-25
 MN1O1    7.33238E-11  SI2      7.96419E-16  C60      1.00000E-30
 C3O2     5.29278E-11  C2       6.41588E-16  O3       1.00000E-30

 FE_LIQUID                    Status ENTERED     Driving force  0.0000E+00
 Moles 2.2343E+04, Mass 1.0734E+06, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.31632E-01  SI  1.89032E-02  O   3.16069E-05
 C   3.93281E-02  MN  1.01049E-02  CA  8.34231E-13

 CA2O2_SIO2                   Status ENTERED     Driving force  0.0000E+00
 Moles 3.5000E+02, Mass 8.6118E+03, Volume fraction 0.0000E+00  Mass fractions:
 CA  4.65382E-01  SI  1.63060E-01  FE  0.00000E+00
 O   3.71558E-01  C   0.00000E+00  MN  0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: save tcex25 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    300.000
 Global calculation of initial equilibrium . impossible due to conditions.
```

```
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    300.000     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  1.10000E+03 .... OK
 Terminating at    2000.00
 Calculated    20 equilibria

 Phase Region from    300.000     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global check of removing phase at  2.02166E+02
 Calculated     3 equilibria

 Phase Region from    202.166     for:
     FE_LIQUID
     CA2O2_SIO2
 Global check of adding phase at  2.00157E+02
 Calculated     3 equilibria

 Phase Region from    200.157     for:
     FE_LIQUID
     CA2O2_SIO2
     CA3O3_SIO2
 Global check of removing phase at  1.66799E+02
 Calculated     4 equilibria

 Phase Region from    166.799     for:
     FE_LIQUID
     CA3O3_SIO2
 Global check of adding phase at  1.66663E+02
 Calculated     3 equilibria

 Phase Region from    166.663     for:
     FE_LIQUID
     CA3O3_SIO2
     CAO
 Terminating at    100.000
 Calculated     4 equilibria
 *** Buffer saved on file: tcex25.POLY3
POLY_3:
POLY_3: @@ The calculations up to 2000 moles is saved on file. At this
POLY_3: @@ point we will change the conditions and start adding scrap in
POLY_3: @@ order to keep the temperature constant. However, the current
POLY_3: @@ equilibrium is at 100 moles of O so we must first make an
POLY_3: @@ interactive calculation at 2000 moles.
POLY_3: read tcex25
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c n(o)
   ... the command in full is SET_CONDITION
Value /300/:  2005
POLY_3: @@ We choose the value a little bigger than 2000 moles as otherwise the
POLY_3: @@ upper limit of the previous calculation coinsides with the lower limit of
POLY_3: @@ this calculation and that will cause trouble
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         2114  grid points in           0  s
    30 ITS,  CPU TIME USED   3 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1948.7315
POLY_3: @@ We now want to keep the temperature constant by adding scrap
POLY_3: @@ Set the temperature as condition
POLY_3: s-c t
   ... the command in full is SET_CONDITION
Value /1948.731455/:
POLY_3:
```

```
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1948.73, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
    N(O)=2005, H=1.32046E9
 DEGREES OF FREEDOM -1
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ we have too many conditions. Assuming the scrap is pure iron we can
POLY_3: @@ just release the condition on the amount of fe.
POLY_3: s-c b(fe)
   ... the command in full is SET_CONDITION
Value /1000000/:  none
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=2005,
    H=1.32046E9
 DEGREES OF FREEDOM 0
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ It is rather special to have both enthalpy
POLY_3: @@ and temperature set as conditions.
POLY_3: @@ We must change the axis limits
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /N(O)/:
Min value /100/:  2000
Max value /2000/:  4000
Increment /50/:  100
POLY_3: @@ We must not give a save command now as that would destroy the
POLY_3: @@ results from the previous step command.
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  normal
 No initial equilibrium, using default
 Step will start from axis value    2005.00
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    2005.00     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  2.80500E+03 .... OK
 Global test at  3.80500E+03 .... OK
 Global check of adding phase at  3.85992E+03
 Calculated    21 equilibria

 Phase Region from    3859.92     for:
     GAS
     FE_LIQUID
     SLAG
     CA2O2_SIO2
 Global check of removing phase at  3.95443E+03
 Calculated     4 equilibria

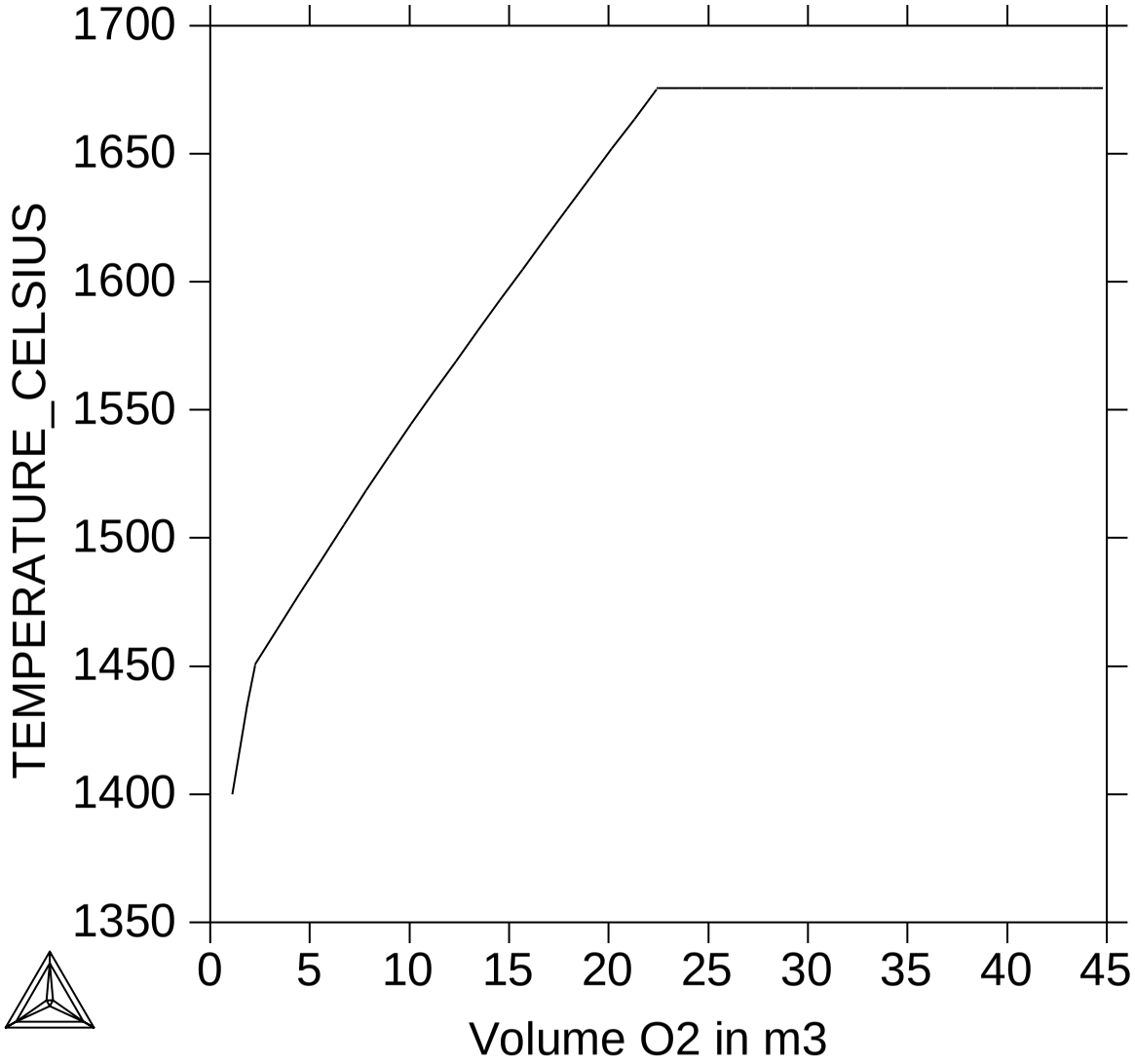
 Phase Region from    3954.43     for:
     GAS
     FE_LIQUID
     SLAG
 Terminating at    4000.00
 Calculated     4 equilibria

 Phase Region from    2005.00     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Terminating at    2000.00
 Calculated     4 equilibria
 *** Buffer saved on file: tcex25.POLY3
POLY_3: no
 No such command, use ?
POLY_3: @@ We shall now plot the combined results
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01
```

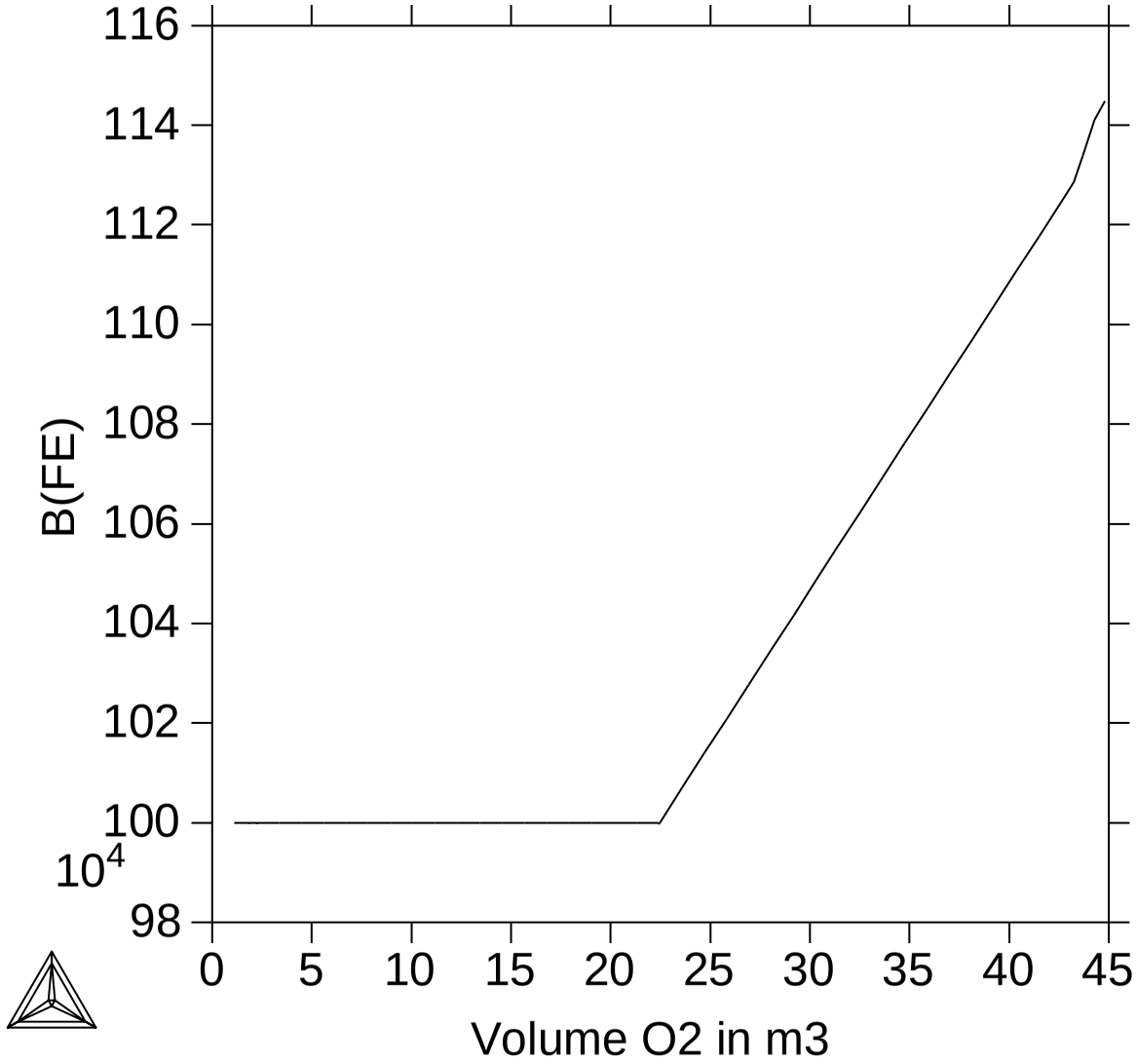
POST: *@@ Use volume of added O2 as independent axis, 1 mole O2 is 0.0224 m3*
POST: *@@ Volume=.0224*(moles of O2)=0.0224*0.5*(moles of O)*
POST: **enter fun vo=0.0112*n(o);**
... the command in full is ENTER_SYMBOL
POST: **s-d-a x vo**
... the command in full is SET_DIAGRAM_AXIS
POST: **s-d-a y t-c**
... the command in full is SET_DIAGRAM_AXIS
POST: *@@ Set a nicer axis text*
POST: **s-a-t-s x n**
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : **Volume O2 in m3**
POST:
POST:
POST: **set-title example 25a**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ Plot the amount of Fe (in grams!)*
POST: **s-d-a y b(fe)**
... the command in full is SET_DIAGRAM_AXIS
POST: **set-title example 25b**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ Plot the mass of all phases*
POST: **s-d-a y bp(*)**
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: **set-lab D**
... the command in full is SET_LABEL_CURVE_OPTION
POST: **set-title example 25c**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ Scale up the slag amount. Liquid slags come at the end only.*
POST: **s-s y n 0 10000**
... the command in full is SET_SCALING_STATUS
POST: **set-title example 25d**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ Now plot the reason for all this -- the steel composition*
POST: **s-d-a y w(fe-l,*)**
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: **set-title example 25e**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ Scale up the diagram to get the important part*
POST: **s-s y n 0 .05**
... the command in full is SET_SCALING_STATUS
POST: **set-title example 25f**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ Finally plot the oxygen partial pressure and carbon activity.*
POST: *@@ For the oxygen plot LN(activity)*
POST: **s-d-a y lnac(o2,gas)**

... the command in full is SET_DIAGRAM_AXIS
POST: **set-lab none**
... the command in full is SET_LABEL_CURVE_OPTION
POST: **set-title example 25g**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST:
POST:
POST: ***@@ For carbon do not forget to set reference state***
POST: **set-ref-state c gra * 1e5**
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: **s-d-a y ac c**
... the command in full is SET_DIAGRAM_AXIS
POST: **set-title example 25h**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST:
POST:
POST: **set-inter**
... the command in full is SET_INTERACTIVE_MODE
POST: CPU time 83 seconds

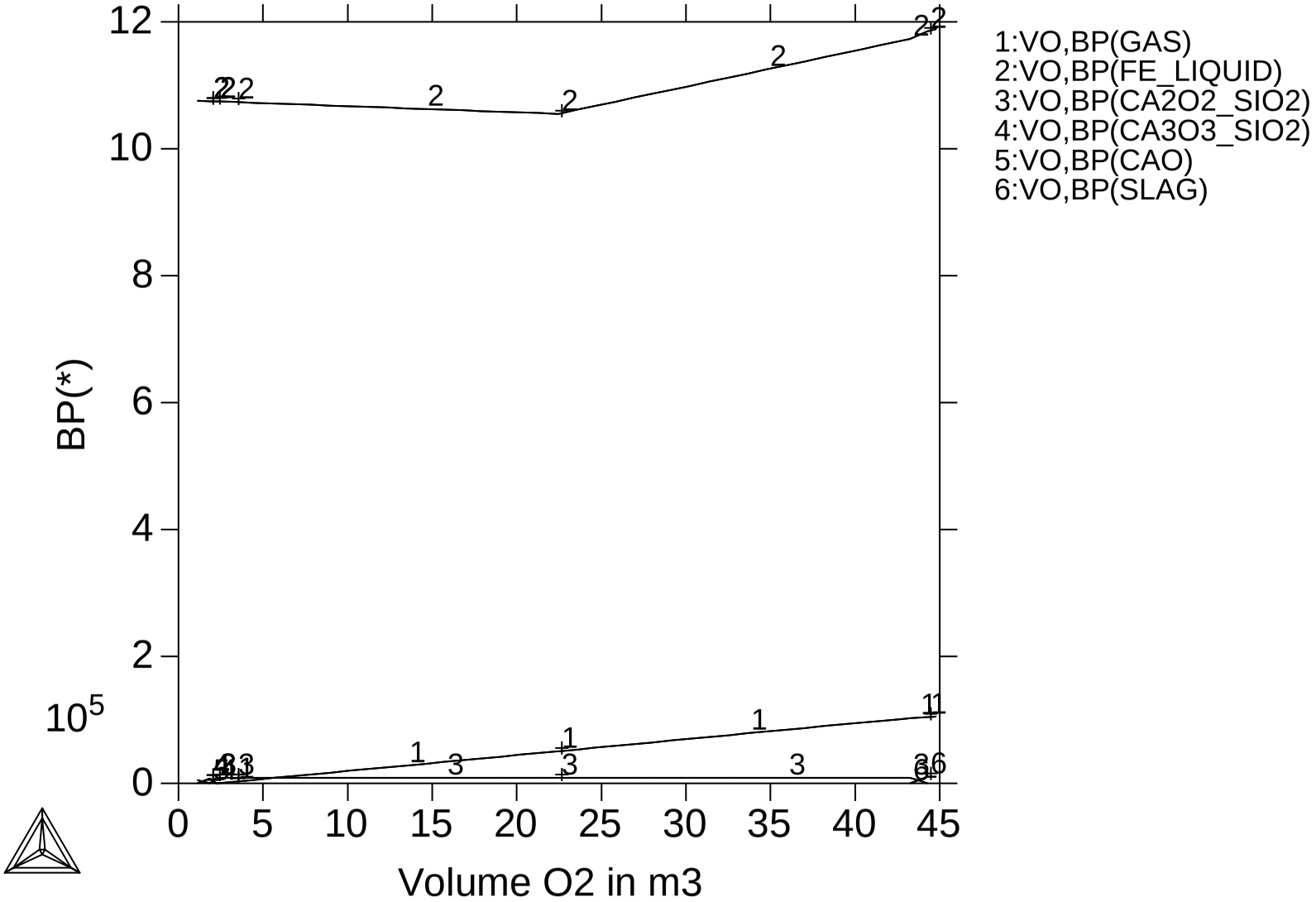
THERMO-CALC (2009.04.15:03.05) :example 25a
DATABASE:SLAG2
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9;



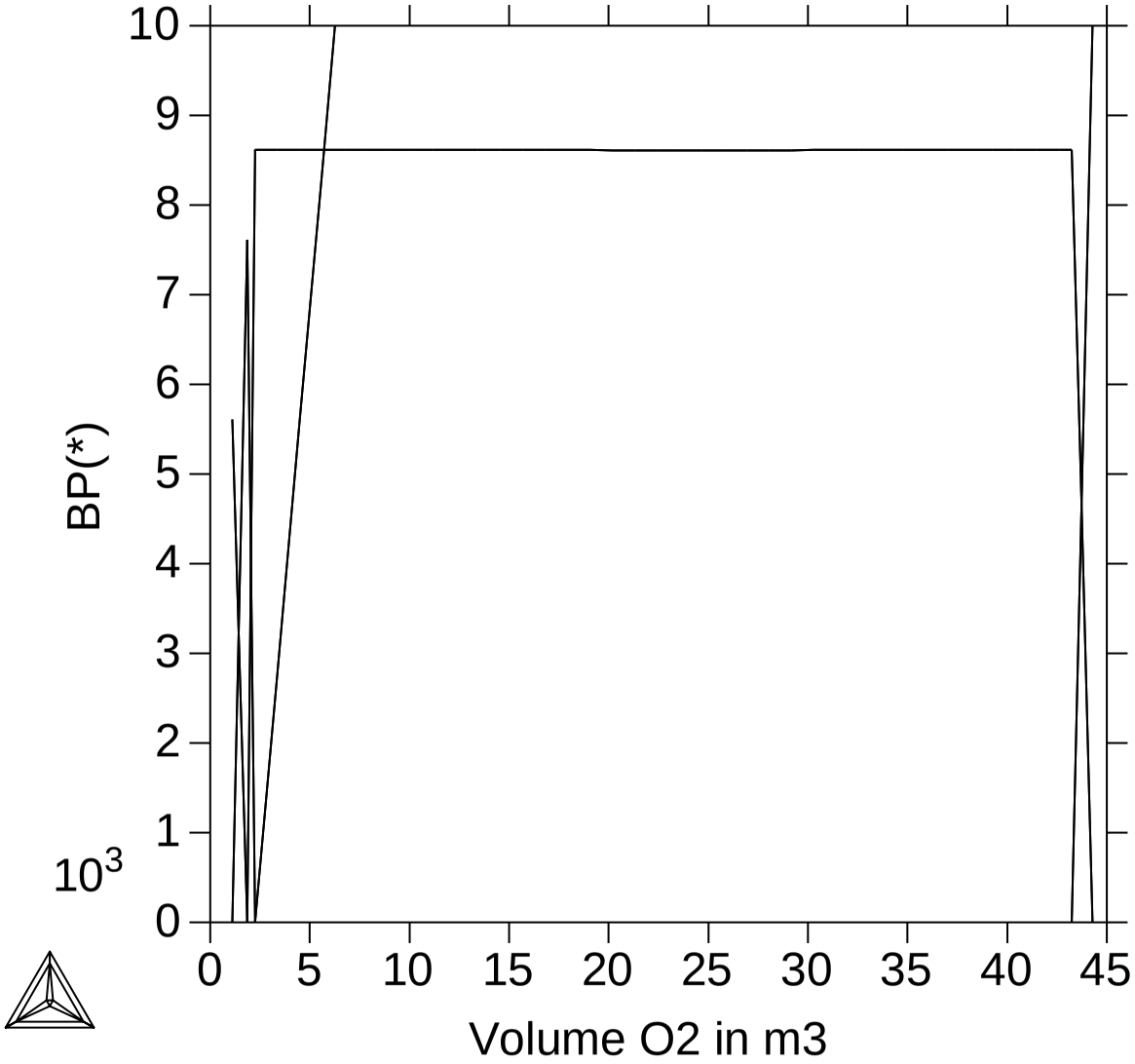
THERMO-CALC (2009.04.15:03.05) :example 25b
DATABASE:SLAG2
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9;



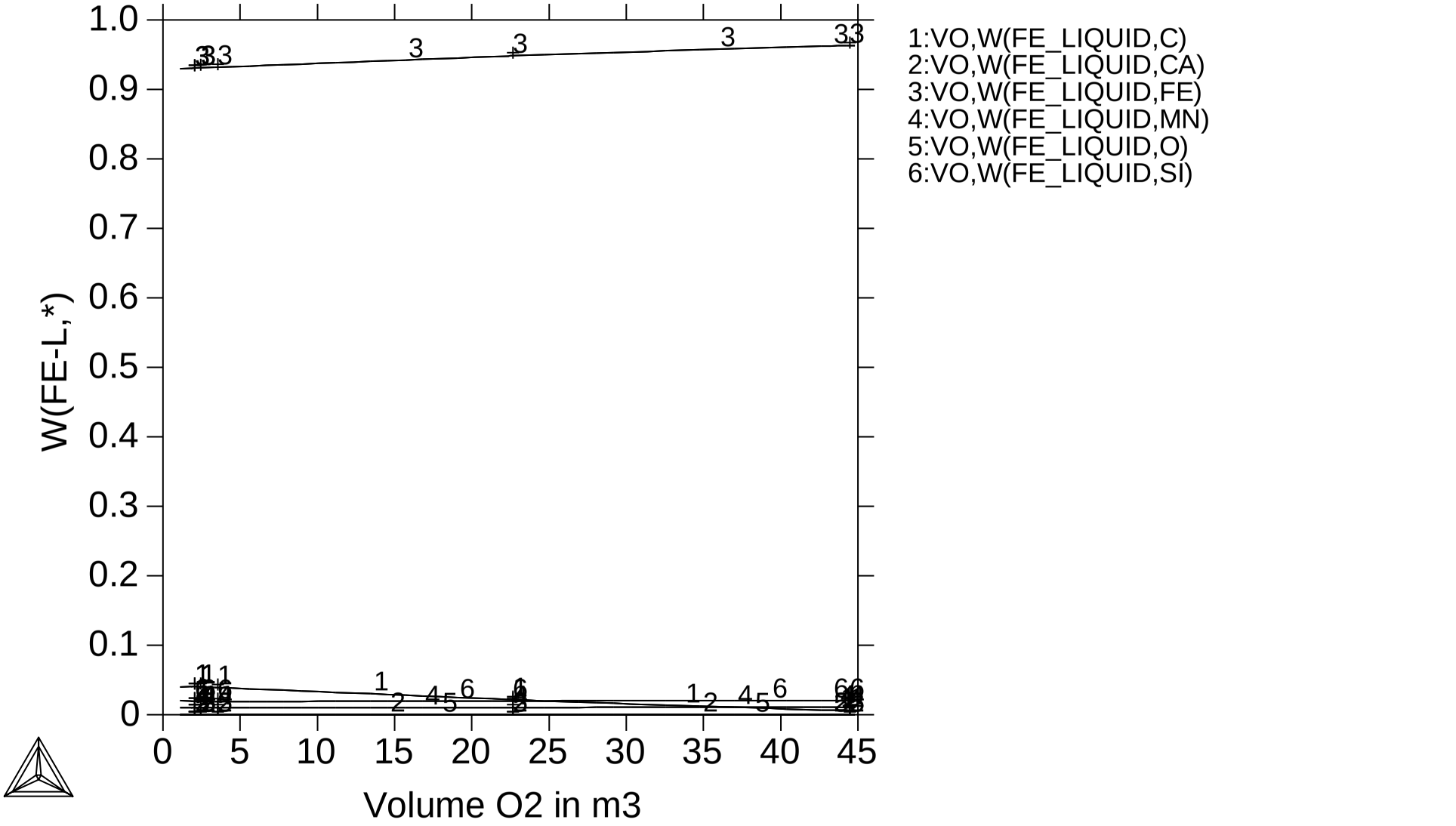
THERMO-CALC (2009.04.15:03.05) :example 25c
DATABASE:SLAG2
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9;



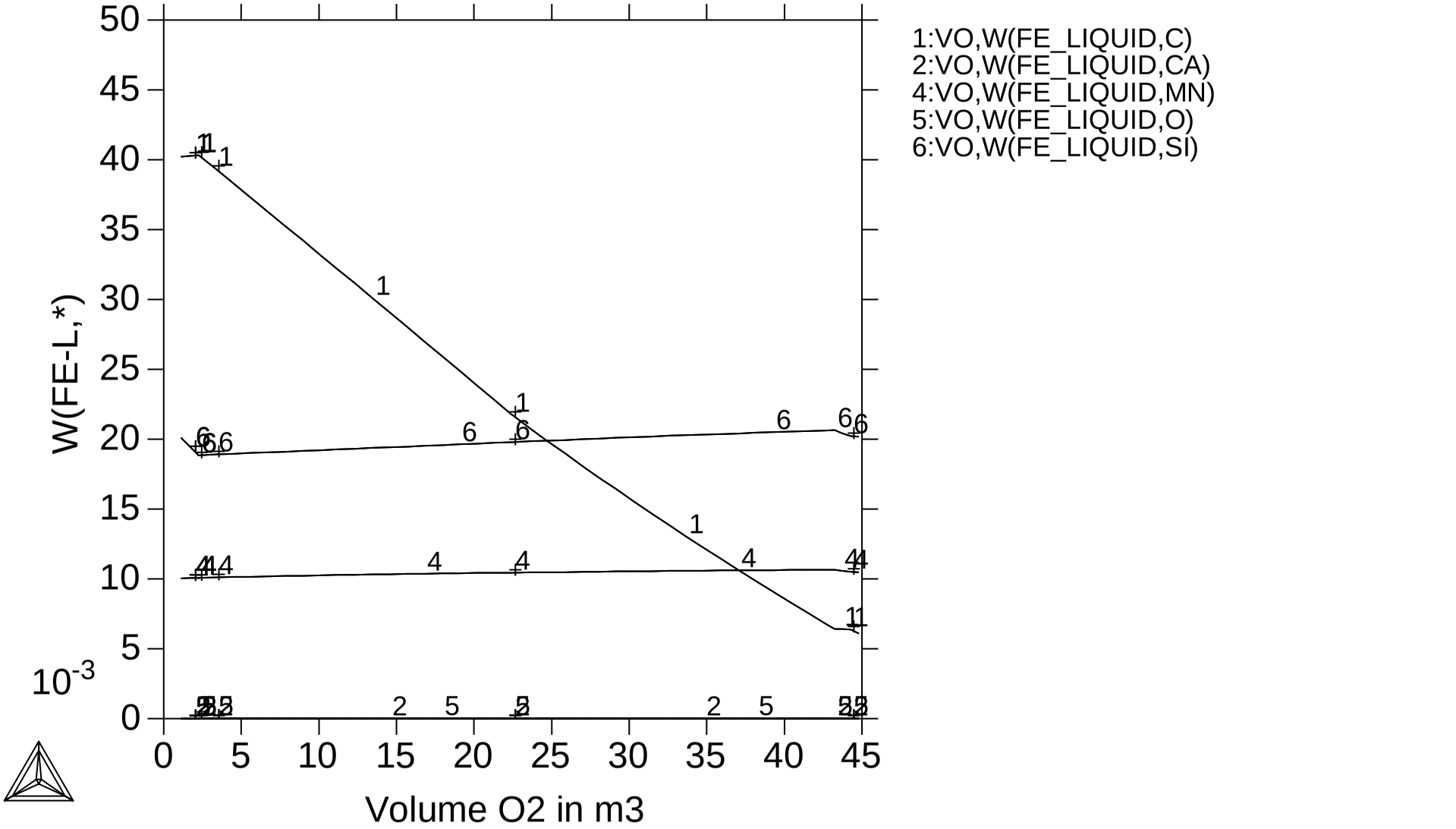
THERMO-CALC (2009.04.15:03.05) :example 25d
DATABASE:SLAG2
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9;



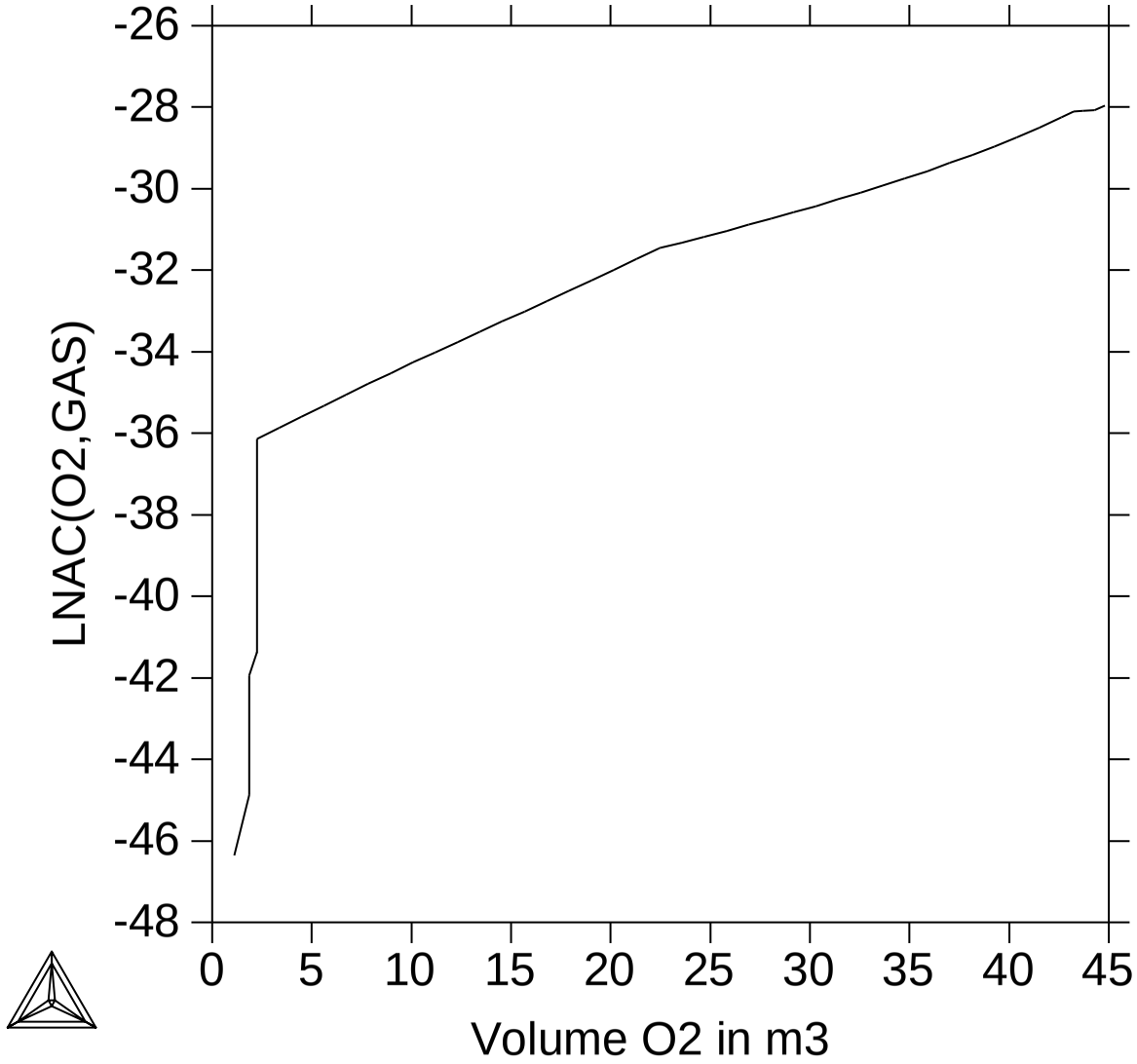
THERMO-CALC (2009.04.15:03.05) :example 25e
DATABASE:SLAG2
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9;



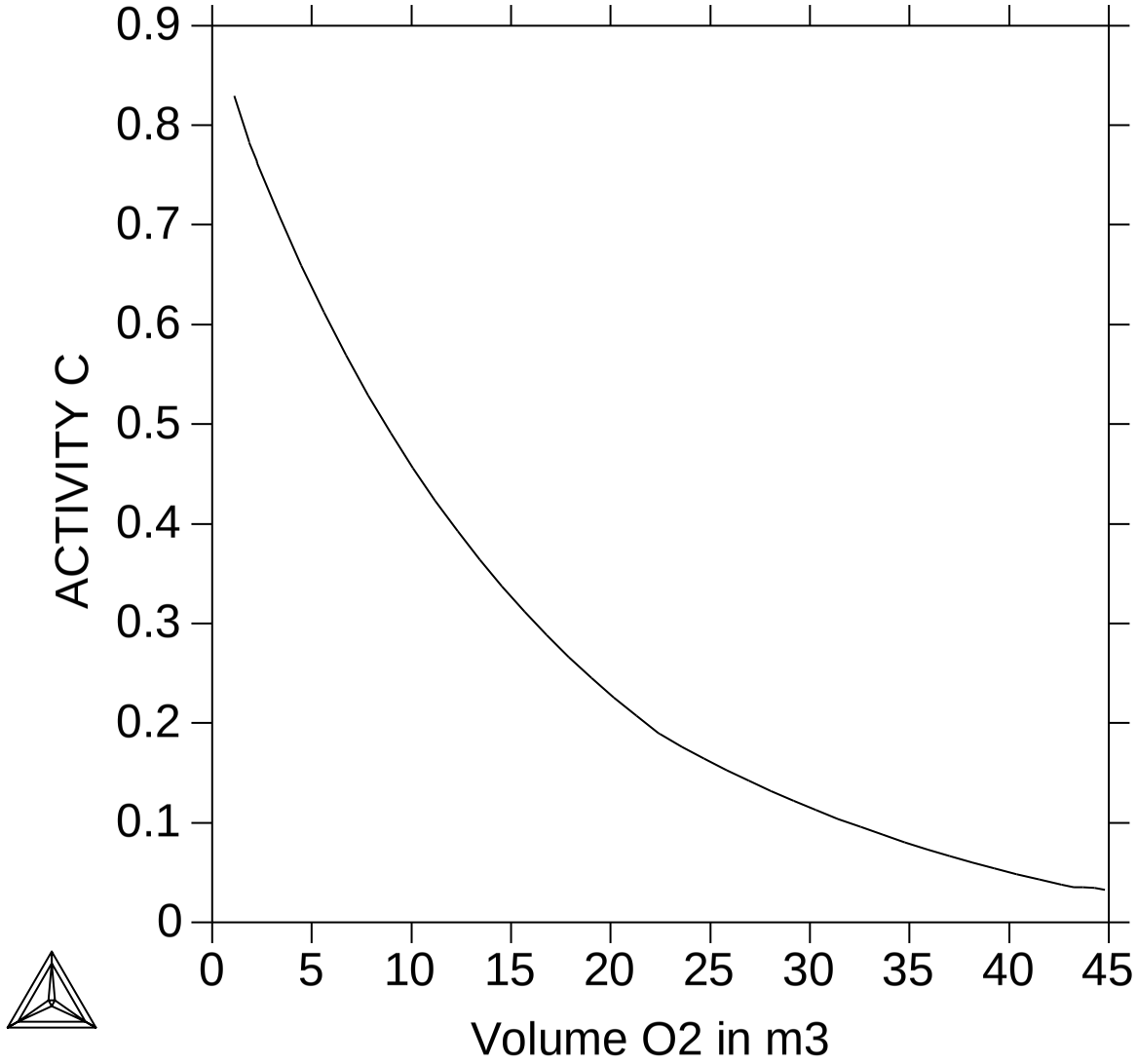
THERMO-CALC (2009.04.15:03.05) :example 25f
DATABASE:SLAG2
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9;



THERMO-CALC (2009.04.15:03.05) :example 25g
DATABASE:SLAG2
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9;



THERMO-CALC (2009.04.15:03.05) :example 25h
DATABASE:SLAG2
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9;



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Plotting of the partial pressure of gas species along the solubility lines in the As-Ga Phase diagram

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example of plotting the partial pressures of a gas along the
SYS: @@ solubility lines in a phase diagram.
SYS: @@ The system is As-Ga.
SYS: @@ The calculation makes it possible to monitor the input gases to
SYS: @@ a process of depositing solid AsGa
SYS: @@
SYS: set-log ex26,,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: @@ At present the data is taken from the special III-V database
TDB_TCFE6: @@ These data will eventually be incorporated in the SGTE solution database
TDB_TCFE6: SW
   ... the command in full is SWITCH_DATABASE
 Use one of these databases

 TCFE6   =  TCS Steels/Fe-Alloys Database v6
 TCFE5   =  TCS Steels/Fe-Alloys Database v5
 TCFE4   =  TCS Steels/Fe-Alloys Database v4
 TCFE3   =  TCS Steels/Fe-Alloys Database v3
 TCFE2   =  TCS Steels/Fe-Alloys Database v2
 TCFE1   =  TCS Steels/Fe-Alloys Database v1
 FEDAT   =  TCS/TT Steels Database v1
 TCNI1   =  TCS Ni-Alloys Database v1
 SSOL4   =  SGTE Alloy Solutions Database v4
 SSOL2   =  SGTE Alloy Solutions Database v2
 SBIN2   =  SGTE Binary Alloys Database v2
 SSUB4   =  SGTE Substances Database v4
 SPOT4   =  SGTE Potential Database v4
 SSUB3   =  SGTE Substances Database v3
 SPOT3   =  SGTE Potential Database v3
 SSUB2   =  SGTE Substances Database v2
 SPOT2   =  SGTE Potential Database v2
 SNOB1   =  SGTE Nobel Metal Alloys Database v2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1
 SALT1   =  SGTE Molten Salt Database v1
 SNUX6   =  SGTE In-Vessel Nuclear Oxide TDB v6.2
 SEMC2   =  TC Semi-Conductors Database v2
 SLAG2   =  TCS Fe-containing Slag Database v2
 SLAG1   =  TCS Fe-containing Slag Database v1
 ION2    =  TCS Ionic Solutions Database v2
 ION1    =  TCS Ionic Solutions Database v1
 NOX2    =  NPL Oxide Solutions Database, v2
 NSLD2   =  NPL Solder Alloys Database v2
 TCMP2   =  TCS Materials Processing Database v2
 TCES1   =  TCS Combustion/Sintering Database v1
 NUMT2   =  TCS Nuclear Materials Database v2
 NUOX4   =  TCS Nuclear Oxides Database v4
 NUTO1   =  TCS U-Zr-Si Ternary Oxides TDB v1
 NUTA1   =  TCS Ag-Cd-In Ternary Alloys TDB v1
 TCNF2   =  TCS Nuclear Fuels Database v2
 TTNI7   =  TT Ni-Alloys Database v7
 TTNI6   =  TT Ni-Alloys Database v6
 TTNI5   =  TT Ni-Alloys Database v5
 TTNF5   =  TT NiFe-Alloys Database v5
 TTTI3   =  TT Ti-Alloys Database v3
 TTTI2   =  TT Ti-Alloys Database v2
 TTTIAL  =  TT TiAl-Alloys Database v1
 TTAL6   =  TT Al-Alloys Database v6
```

```
 TTAL5   =  TT Al-Alloys Database v5
 TTAL4   =  TT Al-Alloys Database v4
 TTAL3   =  TTAL3setup.TDC TT Al-Alloys Database v3
 TTMG4   =  TT Mg-Alloys Database v4
 TTMG3   =  TT Mg-Alloys Database v3
 TTMG2   =  TT Mg-Alloys Database v2
 TTZR1   =  TT Zr-Alloys Database v1
 TCAQ2   =  TCS Aqueous Solution Database v2
 AQS2    =  TGG Aqueous Solution Database v2
 GCE2    =  TGG Geochemical/Environmental TDB v2
 CCC1    =  CCT Cemented Carbides Database v1
 PURE4   =  SGTE Unary (Pure Elements) TDB v4
 PSUB    =  TCS Public Pure Substances TDB v1
 PBIN    =  TCS Public Binary Alloys TDB v1
 PTERN   =  TCS Public Ternary Alloys TDB v1
 PKP     =  Kaufman Binary Alloys TDB v1
 PCHAT   =  Chatenay-Malabry Binary Alloys TDB v1
 PG35    =  G35 Binary Semi-Conductors TDB v1
 PION    =  TCS Public Ionic Solutions TDB v2
 PAQ2    =  TCS Public Aqueous Soln (SIT) TDB v2
 PAQS2   =  TCS Public Aqueous Soln (HKF) TDB v2
 PGEO    =  Saxena Pure Minerals Database v1
 MOB2    =  TCS Alloys Mobility Database v2
 MOB1    =  TCS Alloys Mobility Database v1
 MOBNI1  =  TCS Ni-Alloys Mobility Database v1
 MOBAL1  =  TCS Al-Alloys Mobility Database v1
 BISH    =  Bishop Dilute Al-Alloys MDB v1
 OIKA    =  Oikawa Dilute Fe-Alloys MDB v1
 PFRIB   =  Fridberg Dilute Fe-Alloys MDB v1
 USER    =  User defined Database

DATABASE NAME /TCFE6/: pg35
 Current database: G35 Binary Semi-Conductors TDB v1

 VA  DEFINED
 AL1G                    AL2G                    ALASG
 ALPG                    ALP2G                   ALSBG
   REJECTED
 AS1G                    ASGAG                   ASING
 AS2G                    AS3G                    AS4G
   REJECTED
 GA1G                    GA2G                    GAPG
 GASBG                   GASB2G  REJECTED
 IN1G                    IN2G                    INPG
 INSBG                   INSB2G  REJECTED
 P1G                     P2G                     P4G
 SB1G                    SB2G                    SB3G
 SB4G  REJECTED
TDB_PG35: d-sys as ga
   ... the command in full is DEFINE_SYSTEM
 AS                      GA  DEFINED
TDB_PG35: @@ Reject all but the stable phases in this system
TDB_PG35: rej ph /all
   ... the command in full is REJECT
 GAS:G                   LIQUID                  FCC_A1
 FCC_B3                  BCT_A5                  BCT_A6
 P_RED                   ASP                     RHOMBO_A7
 ORTHO                   GA_GAMMA  REJECTED
TDB_PG35: rest ph liq rhom ortho fcc_b3 gas:g
   ... the command in full is RESTORE
 LIQUID                  RHOMBO_A7               ORTHO
 FCC_B3                  GAS:G  RESTORED
TDB_PG35: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
 GAS:G       :AS1 AS2 AS3 AS4 AS1GA1 GA1 GA2:
  > Gaseous mixture phase: using the Ideal EOS & Mixing Model
 LIQUID      :AS GA:
  > Liquid mixture phase: Metallic species Al-As-Ga-In-P-Sb
 FCC_B3      :GA:AS:
  > FCC_B3 solution phase: for the complete Al-As-Ga-In-P-Sb system
 RHOMBO_A7   :AS:
  > RHOMBO_A7 solution phase: for the As-Sb binary join only
 ORTHO       :GA:
```

```
TDB_PG35: @?<Hit_return_to_continue>
TDB_PG35: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'PG35 - ISC Group III-V Binary Simiconductors Database (V1.2), developed
      by Informal cientific Collaboration Group (Ansara I., Chatillon C.,
      Lukas H.L., Nishizawa T., Ohtani H., Ishida K., Hillert M., Sundman B.,
       Argent B.B., Watson A., Chart T. G., and Anderson T.), 1994, as
      published data [A Binary Database for III-V Compound Semiconductor
      Systems, Calphad, 18, 177-222] and provided by Thermo-Calc Software
      (May 2003/June 2008). '
 -OK-
TDB_PG35: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ Set conditions at the As rich side of the system.
POLY_3: @@ We want to calculate the metastable system whithout gas phase
POLY_3: @@ but later plot the gas constitution. Thus set gas to be dormant.
POLY_3: s-c t=1200 p=1e5 n=1 x(ga)=.3
   ... the command in full is SET_CONDITION
POLY_3: c-s p gas=dor
   ... the command in full is CHANGE_STATUS
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          140  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  x
 Output from POLY-3, equilibrium =     1, label A0  , database: PG35

 Conditions:
 T=1200, P=1E5, N=1, X(GA)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1200.00 K (   926.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  7.33623E+01
 Total Gibbs energy -8.75968E+04,  Enthalpy  1.20850E+04,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 AS                      7.0000E-01  7.0000E-01 1.2211E-03 -6.6929E+04 SER
 GA                      3.0000E-01  3.0000E-01 1.2244E-06 -1.3582E+05 SER

 GAS                         Status DORMANT     Driving force  8.1507E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 AS  1.00000E+00  GA  9.09718E-11
 Constitution:
 AS4     9.80210E-01  AS1     2.30505E-07  GA2     1.87160E-17
 AS2     1.77817E-02  GA1     3.55191E-10
 AS3     2.00768E-03  AS1GA1  5.27773E-12

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.0575E-01, Mass 3.7617E+01, Volume fraction 0.0000E+00  Mole fractions:
 AS  8.95449E-01  GA  1.04551E-01

 FCC_B3                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.9425E-01, Mass 3.5745E+01, Volume fraction 0.0000E+00  Mole fractions:
 AS  5.00000E-01  GA  5.00000E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Note that the gas would like to be stable (driving force positive)
POLY_3: @@ but it is not allowed to form as it is dormant.
POLY_3: l-st ph
```

```
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 LIQUID                 ENTERED    0.00000000E+00  5.05753875E-01
 FCC_B3                 ENTERED    0.00000000E+00  4.94246125E-01
 RHOMBO_A7              ENTERED   -4.05904476E-01  0.00000000E+00
 ORTHO                  ENTERED   -6.64422975E+00  0.00000000E+00
 GAS                    DORMANT    8.15065838E-01
POLY_3: @@ The phase diagram is calculated with the composition and
POLY_3: @@ temperature on the axis as usual
POLY_3: s-a-v 1 x(ga)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  1
Increment /.025/:  .025
POLY_3: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  300
Max value /1/:  2000
Increment /42.5/:  25
POLY_3: @@ For an explanation of these symbols see below
POLY_3: ent fun pas1=0.4343*lnacr(as1,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas2=0.4343*lnacr(as2,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas3=0.4343*lnacr(as3,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas4=0.4343*lnacr(as4,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pasga=0.4343*lnacr(as1ga1,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun pga1=0.4343*lnacr(ga1,gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent tab pp
   ... the command in full is ENTER_SYMBOL
Variable(s): pas1 pas2 pas3 pas4 pasga pga1;
POLY_3:
POLY_3: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED FUNCTIONS AND VARIABLES%
    PAS1=.4343*LNACR(AS1,GAS)
    PAS2=.4343*LNACR(AS2,GAS)
    PAS3=.4343*LNACR(AS3,GAS)
    PAS4=.4343*LNACR(AS4,GAS)
    PASGA=.4343*LNACR(AS1GA1,GAS)
    PGA1=.4343*LNACR(GA1,GAS)
 DEFINED TABLES
    PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
POLY_3: @?<Hit_return_to_continue>
POLY_3: ent fun dd=0.4343*dgf(gas);
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas1=log10(y(gas,as1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas2=log10(y(gas,as2))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas3=log10(y(gas,as3))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas4=log10(y(gas,as4))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qasga=log10(y(gas,as1ga1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent fun qga1=log10(y(gas,ga1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent tab qq
   ... the command in full is ENTER_SYMBOL
Variable(s): qas1 qas2 qas3 qas4 qasga qga1;
POLY_3:
POLY_3: ent fun it=1000/T;
   ... the command in full is ENTER_SYMBOL
POLY_3: save tcex26 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED FUNCTIONS AND VARIABLES%
```

```
    PAS1=.4343*LNACR(AS1,GAS)
    PAS2=.4343*LNACR(AS2,GAS)
    PAS3=.4343*LNACR(AS3,GAS)
    PAS4=.4343*LNACR(AS4,GAS)
    PASGA=.4343*LNACR(AS1GA1,GAS)
    PGA1=.4343*LNACR(GA1,GAS)
    DD=.4343*DGF(GAS)
    QAS1= LOG10(Y(GAS,AS1) )+DD
    QAS2= LOG10(Y(GAS,AS2) )+DD
    QAS3= LOG10(Y(GAS,AS3) )+DD
    QAS4= LOG10(Y(GAS,AS4) )+DD
    QASGA= LOG10(Y(GAS,AS1GA1) )+DD
    QGA1= LOG10(Y(GAS,GA1) )+DD
    IT=1000/T
 DEFINED TABLES
    PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
    QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Map follows all lines in the phase diagram
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   2.500E-01  3.100E+02
  ** FCC_B3
     RHOMBO_A7
 *** Buffer saved on file: tcex26.POLY3
 Calculated..            2  equilibria
```

```
 Terminating at axis limit.

 Phase region boundary   2 at:   2.500E-01  3.000E+02
  ** FCC_B3
     RHOMBO_A7
 Calculated.           32  equilibria

 Phase region boundary   3 at:   2.500E-01  1.067E+03
  ** FCC_B3
  ** LIQUID
     RHOMBO_A7

 Phase region boundary   4 at:   2.345E-02  1.067E+03
  ** LIQUID
     RHOMBO_A7
 Calculated           10  equilibria

       :
       :
       :

 Phase region boundary  32 at:   5.817E-01  1.468E+03
  ** FCC_B3
     LIQUID
 Calculated.           34  equilibria
 Terminating at known equilibrium

 Phase region boundary  33 at:   5.817E-01  1.468E+03
  ** FCC_B3
     LIQUID
 Calculated.           54  equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   7.450E-01  9.995E+02
  ** FCC_B3
     LIQUID
 Calculated.           74  equilibria
 Terminating at known equilibrium

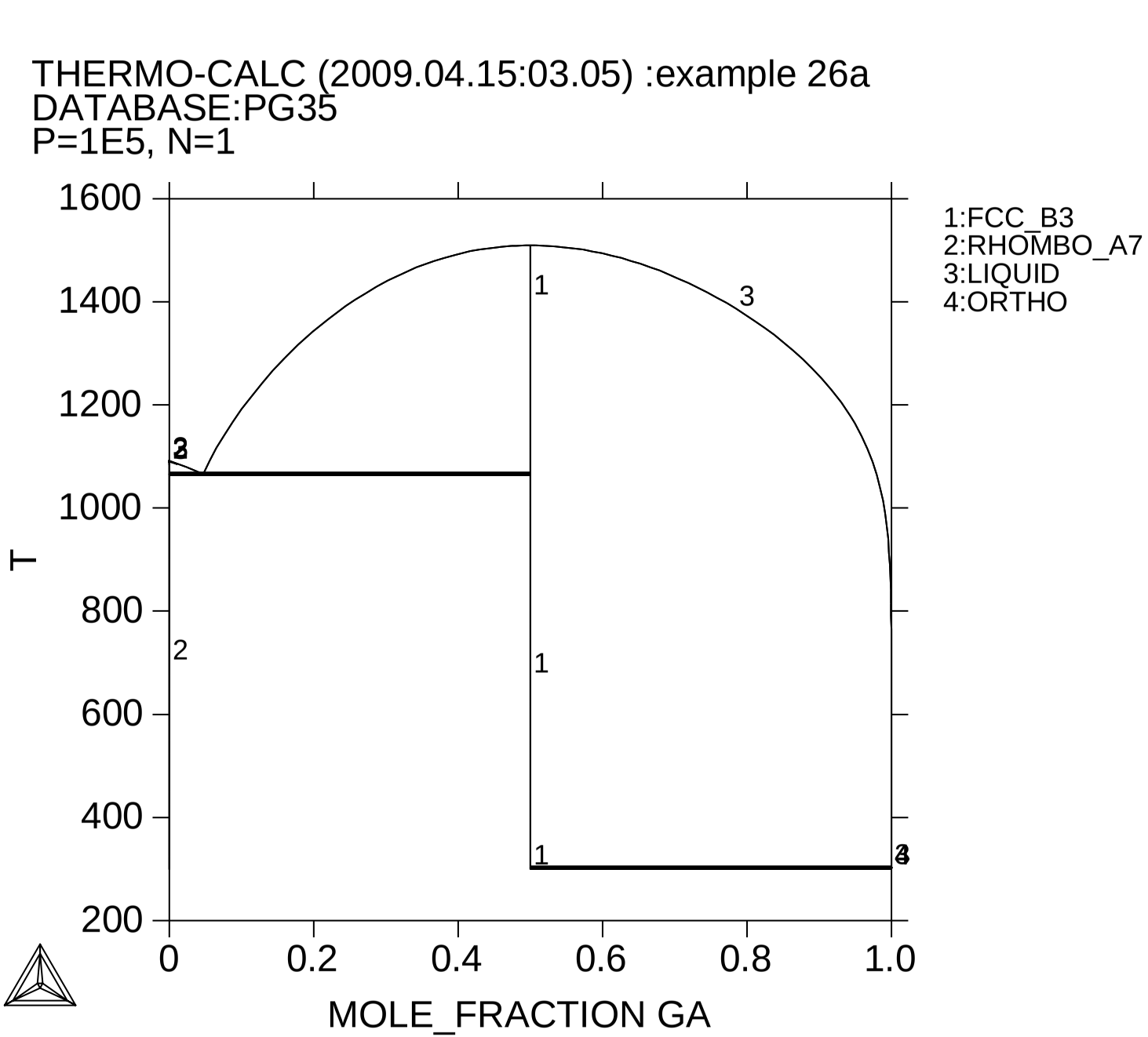
 Phase region boundary  35 at:   7.450E-01  9.995E+02
  ** FCC_B3
     LIQUID
 Calculated.           29  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex26.POLY3
 CPU time for mapping          2  seconds
POLY_3: @@ Now we plot this in the post processor
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

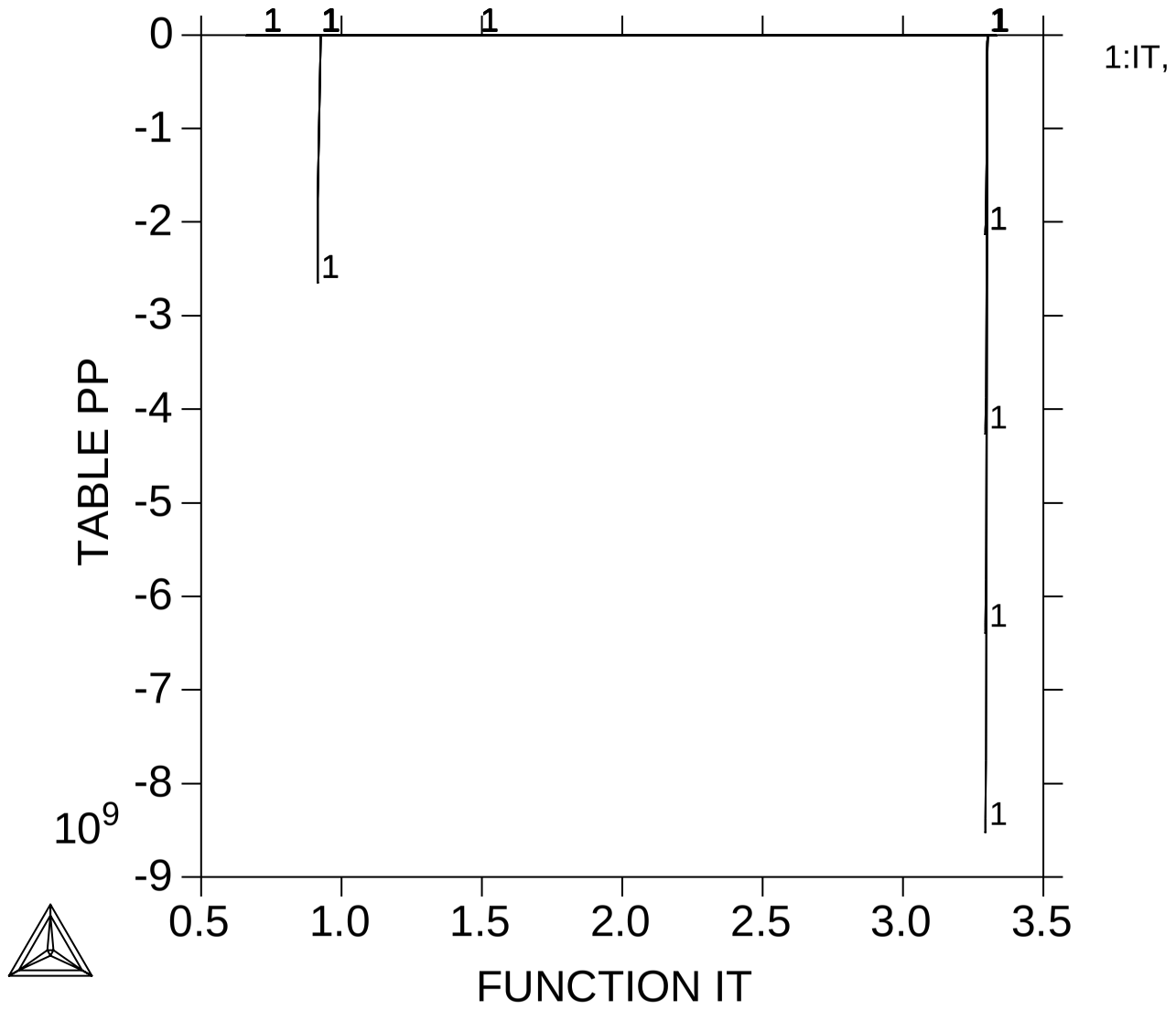
 Setting automatic diagram axis

POST: s-d-a x m-f ga
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 26a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ This is the traditional phase diagram.
POST: @@
POST: @@ Now those who work with this system is interested to know the
POST: @@ partial pressures of the different gas species along the
POST: @@ solubility lines. As Thermo-Calc saves the complete description of
POST: @@ all tie-lines calculated in a MAP or STEP command, even for
POST: @@ dormat phases, we can now plot these.
```

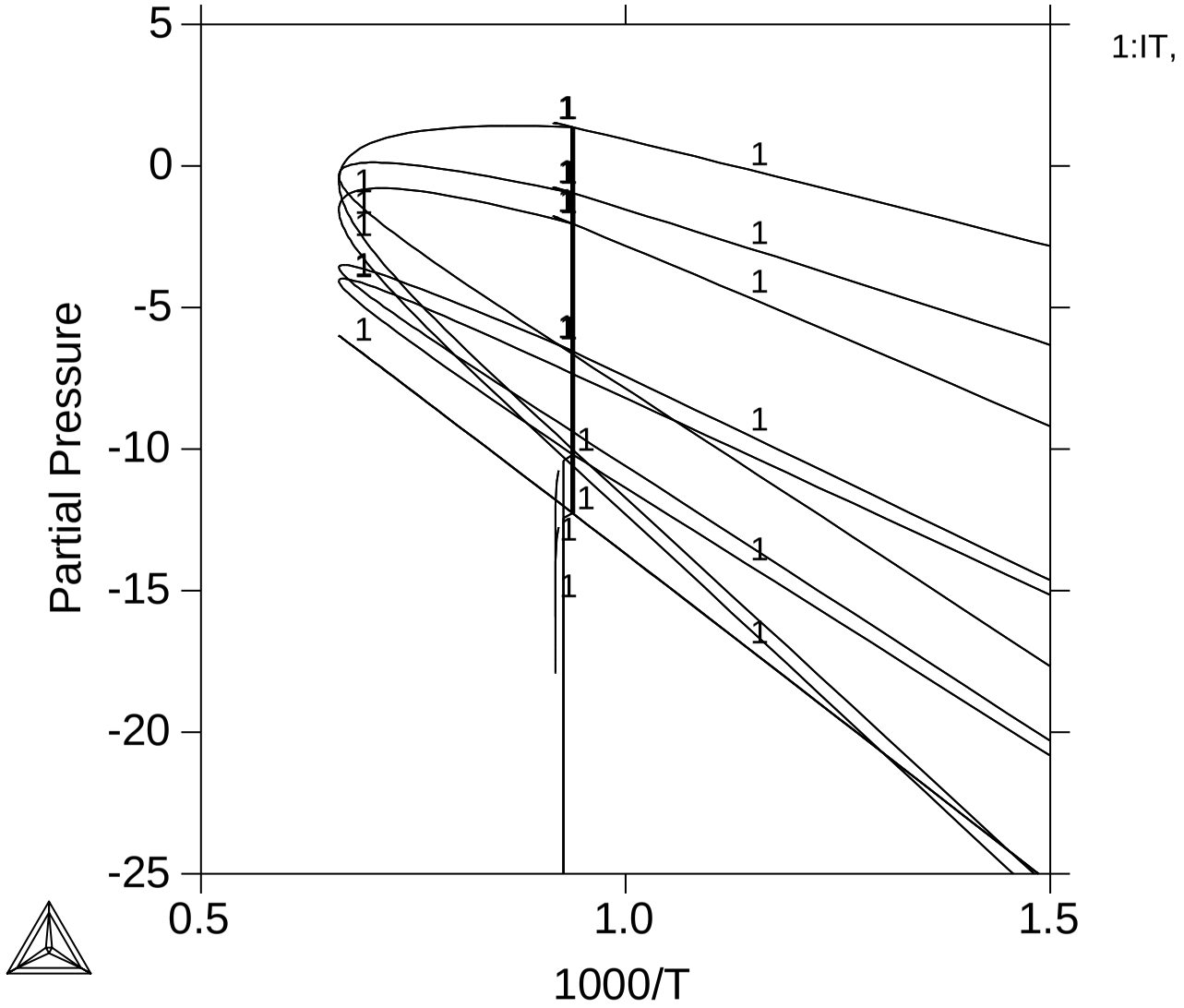
POST: **@@ The partial pressures of a species in the gas is equal to the**
POST: **@@ fraction of that species if the gas is stable (Dalton's law)**
POST: **@@ If the gas is not stable one must add the driving force per**
POST: **@@ formula unit of the gas (the formula unit depends on the species)**
POST: **@@**
POST: **@@ We can obtain directly the activity of a gas species using the**
POST: **@@ state variable acr(species,gas) which will have as**
POST: **@@ reference state a pure gas of the species itself. The state variable**
POST: **@@ lnacr(species,gas) is the natural logarithm of this quantity. To make**
POST: **@@ it into log10 one must multiply by 0.4343**
POST: **@@**
POST: **s-d-a y pp**
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: **@@ plot againt the inverse of temperature**
POST: **s-d-a x it**
... the command in full is SET_DIAGRAM_AXIS
POST: **l-sy**
... the command in full is LIST_SYMBOLS
```
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    PAS1=.4343*LNACR(AS1,GAS)
    PAS2=.4343*LNACR(AS2,GAS)
    PAS3=.4343*LNACR(AS3,GAS)
    PAS4=.4343*LNACR(AS4,GAS)
    PASGA=.4343*LNACR(AS1GA1,GAS)
    PGA1=.4343*LNACR(GA1,GAS)
    DD=.4343*DGF(GAS)
    QAS1= LOG10(Y(GAS,AS1) )+DD
    QAS2= LOG10(Y(GAS,AS2) )+DD
    QAS3= LOG10(Y(GAS,AS3) )+DD
    QAS4= LOG10(Y(GAS,AS4) )+DD
    QASGA= LOG10(Y(GAS,AS1GA1) )+DD
    QGA1= LOG10(Y(GAS,GA1) )+DD
    IT=1000/T
    TEMP_C=T-273.15
 DEFINED TABLES
    PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
    QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
```
POST: **set-title example 26b**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **@@ Now make the plot readable by adding axis text and labels**
POST: **s-s x n 0.5 1.5**
... the command in full is SET_SCALING_STATUS
POST: **s-s y n -25 5**
... the command in full is SET_SCALING_STATUS
POST: **s-a-text x n 1000/T**
... the command in full is SET_AXIS_TEXT_STATUS
POST: **s-a-text y n Partial Pressure**
... the command in full is SET_AXIS_TEXT_STATUS
POST: **s-lab d**
... the command in full is SET_LABEL_CURVE_OPTION
POST: **set-title example 26c**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **set-interactive**
... the command in full is SET_INTERACTIVE_MODE
POST: CPU time 2 seconds


THERMO-CALC (2009.04.15:03.05) :example 26a
DATABASE:PG35
P=1E5, N=1
1600
1400
1200
1000
800
600
400
200
T
0
0.2
0.4
0.6
0.8
1.0
MOLE_FRACTION GA
1
2
3
1
2
1
1
3
1:FCC_B3
2:RHOMBO_A7
3:LIQUID
4:ORTHO

THERMO-CALC (2009.04.15:03.05) :example 26b
DATABASE:PG35
P=1E5, N=1



THERMO-CALC (2009.04.15:03.05) :example 26c
DATABASE:PG35
P=1E5, N=1



27

CVD calculations

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example of CVD calculation
SYS: @@
SYS: @@
SYS: @@ Get data from database
SYS: set-log ex27,,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw ssub4
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v4

 VA  DEFINED
TDB_SSUB4:
TDB_SSUB4: d-sys h cl ar w si
   ... the command in full is DEFINE_SYSTEM
 H                       CL                      AR
 W                       SI  DEFINED
TDB_SSUB4: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   AR1<G> HULTGREN SELECTED VAL 1973 SGTE **
      ARGON <GAS>
      STANDARD STATE : CODATA KEY VALUE .
   CL1<G> T.C.R.A.S. Class: 1
      CHLORINE <MONATOMIC GAS>
   CL10W2<G> JANAF THERMOCHEMICAL TABLES SGTE
      TUNGSTEN PENTACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
                    :
                    :
                    :
   SI2W1 VAHLAS ET AL **
      from Vahlas et al Calphad 13(3) (1989) 273
   SI3W5 VAHLAS ET AL **
      from Vahlas et al Calphad 13(3) (1989) 273
   SI1 JANAF THERMOCHEMICAL TABLES SGTE **
      SILICON
      PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
      --U.D. 31/10/85
   W1 S.G.T.E. **
      Data from SGTE Unary DB
 -OK-
TDB_SSUB4: @@
TDB_SSUB4: @@ Calculations are made in POLY-3 module
TDB_SSUB4: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@
POLY_3: @@ In poly-3 you define new components
```

```
POLY_3: def-com ar cl4w1 cl2h2si1 h2 cl1h1
   ... the command in full is DEFINE_COMPONENTS
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT              STATUS    REF. STATE     T(K)          P(Pa)
 VA                     ENTERED   SER
 AR                     ENTERED   SER
 CL4W1                  ENTERED   SER
 CL2H2SI1               ENTERED   SER
 H2                     ENTERED   SER
 CL1H1                  ENTERED   SER
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@
POLY_3: @@ Set conditions for input of gases. This may be tricky. The best
POLY_3: @@ is probably to set amounts equal to moles/minutes or something
POLY_3: @@ like that. In this case we had initial partial pressures of
POLY_3: @@ argon 0.9 atm, WCL4 1e-5..0.1 SiH2Cl2 1e-5..0.1 unkown presure of H2
POLY_3: @@ and no addition of HCl nor Cl (?).
POLY_3: s-c n=1 x(ar)=.9 x(cl2h2si)=1e-3 x(cl4w)=.001 x(cl1h1)=0
   ... the command in full is SET_CONDITION
POLY_3: @@
POLY_3: @@ At the reaction zone T=1000 and total pressure is 1 atm
POLY_3: s-c t=1000 p=101325
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=0, T=1000,
    P=1.01325E5
 DEGREES OF FREEDOM 0
POLY_3: @@
POLY_3: @@ Save what we have done so far on a file if something happens ...
POLY_3: @@ and then calculate and list the results
POLY_3: save tcex27 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          481  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Global minimization failed, error code         1611 TOO MANY ITERATIONS

 *** ERROR  1611 IN QEQUIL
 *** TOO MANY ITERATIONS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB4

 Conditions:
 N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=0, T=1000,
    P=1.01325E5
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.013250E+05
 Number of moles of components  5.08355E-01,  Mass in grams  8.53863E+01
 Total Gibbs energy -5.06128E+05,  Enthalpy -2.96135E+05,  Volume  7.75585E-04

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AR                      1.2560E-03  5.8763E-04 3.5067E-10 -1.8102E+05 SER
 CL4W1                   1.1057E-04  4.2170E-04 2.4677E-35 -6.6256E+05 SER
 CL2H2SI1                5.0157E-01  5.9333E-01 2.0168E-32 -6.0680E+05 SER
 H2                     -9.9986E-01 -2.3605E-02 1.0189E-14 -2.6787E+05 SER
 CL1H1                   1.0053E+00  4.2927E-01 8.8267E-16 -2.8821E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 9.4511E-03, Mass 5.8493E-01, Volume fraction 1.0000E+00  Mass fractions:
 CL1H1     4.79508E-01  AR        8.57801E-02  H2       -7.08537E-03
 CL2H2SI1  4.41797E-01  CL4W1     1.14458E-08
 Constitution:
 CL1H1     5.11269E-01  CL1H1SI1  6.60399E-09  CL5W1     3.38354E-16
 CL3H1SI1  2.35693E-01  CL        3.80577E-09  H1SI1     1.38814E-17
 AR        1.32889E-01  CL2W1     2.17063E-09  SI        2.21529E-19
```

```
 H2        8.51549E-02  CL1SI1    2.93995E-10  H6SI2     4.70248E-20
 CL4SI1    3.39191E-02  H4SI1     2.53727E-11  CL6W1     3.16641E-21
 CL1H3SI1  9.12922E-04  CL4W1     4.44365E-12  SI2       6.97149E-25
 CL2H2SI1  1.00138E-04  CL2       8.62565E-13  CL10W2    1.11230E-26
 CL2SI1    6.18887E-05  CL3W1     2.96272E-15  CL1W1     2.07876E-28
 CL3SI1    6.29810E-07  H3SI1     1.84887E-15  SI3       1.72538E-28
 H         1.76159E-08  H2SI1     1.43029E-15  W         1.95131E-29

 CL4SI1_L                    Status ENTERED     Driving force  4.3124E+01
 Moles 4.9901E-01, Mass 8.4781E+01, Volume fraction 0.0000E+00  Mass fractions:
 CL2H2SI1  5.94518E-01  AR        0.00000E+00  H2       -2.37297E-02
 CL1H1     4.29212E-01  CL4W1     0.00000E+00

 W_S                         Status ENTERED     Driving force  0.0000E+00
 Moles-1.1057E-04, Mass 2.0328E-02, Volume fraction 0.0000E+00  Mass fractions:
 CL4W1     1.77135E+00  AR        0.00000E+00  CL1H1    -7.93275E-01
 H2        2.19287E-02  CL2H2SI1  0.00000E+00

 SI_S                        Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CL2H2SI1  3.59647E+00  H2        0.00000E+00  CL1H1    -2.59647E+00
 AR        0.00000E+00  CL4W1     0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ To get into the single phase Si3W5 area, reduce x(cl4w1) a little
POLY_3: s-c x(cl4w1)=.0008
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB4

 Conditions:
 N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=8E-4, X(CL1H1)=0, T=1000,
    P=1.01325E5
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  3.65127E+01
 Total Gibbs energy -1.67377E+05,  Enthalpy  1.46284E+04,  Volume  8.21629E-02

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AR                      9.0000E-01  9.8468E-01 2.0874E-09 -1.6618E+05 SER
 CL4W1                   8.0000E-04  7.1353E-03 1.0761E-57 -1.0906E+06 SER
 CL2H2SI1                1.0000E-03  2.7663E-03 3.4267E-40 -7.5555E+05 SER
 H2                      9.8200E-02  5.4214E-03 2.4680E-09 -1.6479E+05 SER
 CL1H1                   1.2901E-15  1.2892E-15 1.4363E-18 -3.4160E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0013E+00, Mass 3.6352E+01, Volume fraction 1.0000E+00  Mass fractions:
 AR        9.89026E-01  CL1H1     4.17245E-03  CL4W1     2.95978E-11
 H2        5.35667E-03  CL2H2SI1  1.44485E-03
 Constitution:
 AR        8.98849E-01  CL1H1SI1  6.93792E-11  CL3W1     2.66476E-18
 H2        9.73448E-02  H4SI1     2.57317E-11  SI        1.13381E-18
 CL1H1     3.28695E-03  CL        2.21191E-11  H6SI2     2.46912E-21
 CL4SI1    3.76481E-04  CL1SI1    4.32956E-12  CL5W1     3.83423E-25
 CL3H1SI1  1.28086E-04  CL2W1     3.29962E-12  SI2       2.22686E-25
 CL1H3SI1  1.33248E-05  CL2       3.27970E-15  SI3       8.54134E-29
 CL2H2SI1  7.88802E-07  H3SI1     1.79309E-15  W         1.00000E-30
 CL2SI1    6.48597E-07  H2SI1     1.60803E-15  CL1W1     1.00000E-30
 CL3SI1    5.37497E-09  H1SI1     6.51082E-17  CL10W2    1.00000E-30
 H         7.04089E-10  CL4W1     1.35122E-17  CL6W1     1.00000E-30

 SI3W5_S                     Status ENTERED     Driving force  0.0000E+00
 Moles-1.2800E-03, Mass 1.6056E-01, Volume fraction 0.0000E+00  Mass fractions:
 CL4W1     1.62262E+00  H2        2.00876E-02  CL1H1    -9.44672E-01
 CL2H2SI1  3.01962E-01  AR        0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@
```

```
POLY_3: @@ Now set axis to vary along the input amounts of WCl4 and SiH2Cl2.
POLY_3: @@ Use logarithmic step as the magnitudes varies a lot.
POLY_3: @@ Note that a limit equal to zero should not be used with log.axis!
POLY_3: s-a-v 1 x(cl2h2si)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  1e-8
Max value /1/:  0.02
Increment /4.9999975E-04/:  2.0*
 Logarithmic step set
POLY_3: s-a-v 2 x(cl4w)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  1e-8
Max value /1/:  0.02
Increment /4.9999975E-04/:  2.0*
 Logarithmic step set
POLY_3: @@ Add with both direction and continuation ">" to be sure to get all lines
POLY_3: add
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
Direction /Default/: 2>
POLY_3: add -2>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: l-ax
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: X(CL2H2SI1)          Min: 1E-8      Max: 2E-2      Inc: 2*
  Axis No 2: X(CL4W1)             Min: 1E-8      Max: 2E-2      Inc: 2*
POLY_3: li-in
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  +2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=8E-4,
    X(CL1H1)=1.3550901E-15, T=1000, P=101325
 No 2  -2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=8E-4,
    X(CL1H1)=1.3503196E-15, T=1000, P=101325
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@
POLY_3: @@ save again with the start point before mapping
POLY_3: save tcex27 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18

 Phase region boundary   1 at:   1.435E-02  1.970E-03
     GAS
     SI2W1_S
  ** SI_S
 *** Buffer saved on file: tcex27.POLY3
 Calculated           70  equilibria

 Phase region boundary   2 at:   1.435E-02  1.970E-03
     GAS
     SI2W1_S
```

```
 ** SI_S
 Calculated..            2  equilibria
 Terminating at axis limit.

 Phase region boundary   3 at:   2.000E-02  2.810E-03
     GAS
     SI2W1_S
  ** SI_S
 Calculated           71  equilibria

 Phase region boundary   4 at:   9.344E-03  1.970E-03
     GAS
     SI2W1_S
  ** SI3W5_S
 Calculated           94  equilibria

       :
       :
       :

 Phase region boundary  20 at:   1.000E-03  3.753E-04
     GAS
     SI2W1_S
  ** SI3W5_S
 Calculated           33  equilibria

 Phase region boundary  21 at:   1.000E-03  3.753E-04
     GAS
     SI2W1_S
  ** SI3W5_S
 Calculated..            6  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  22 at:   1.000E-03  7.855E-04
     GAS
  ** SI2W1_S
     SI3W5_S
 Calculated           33  equilibria

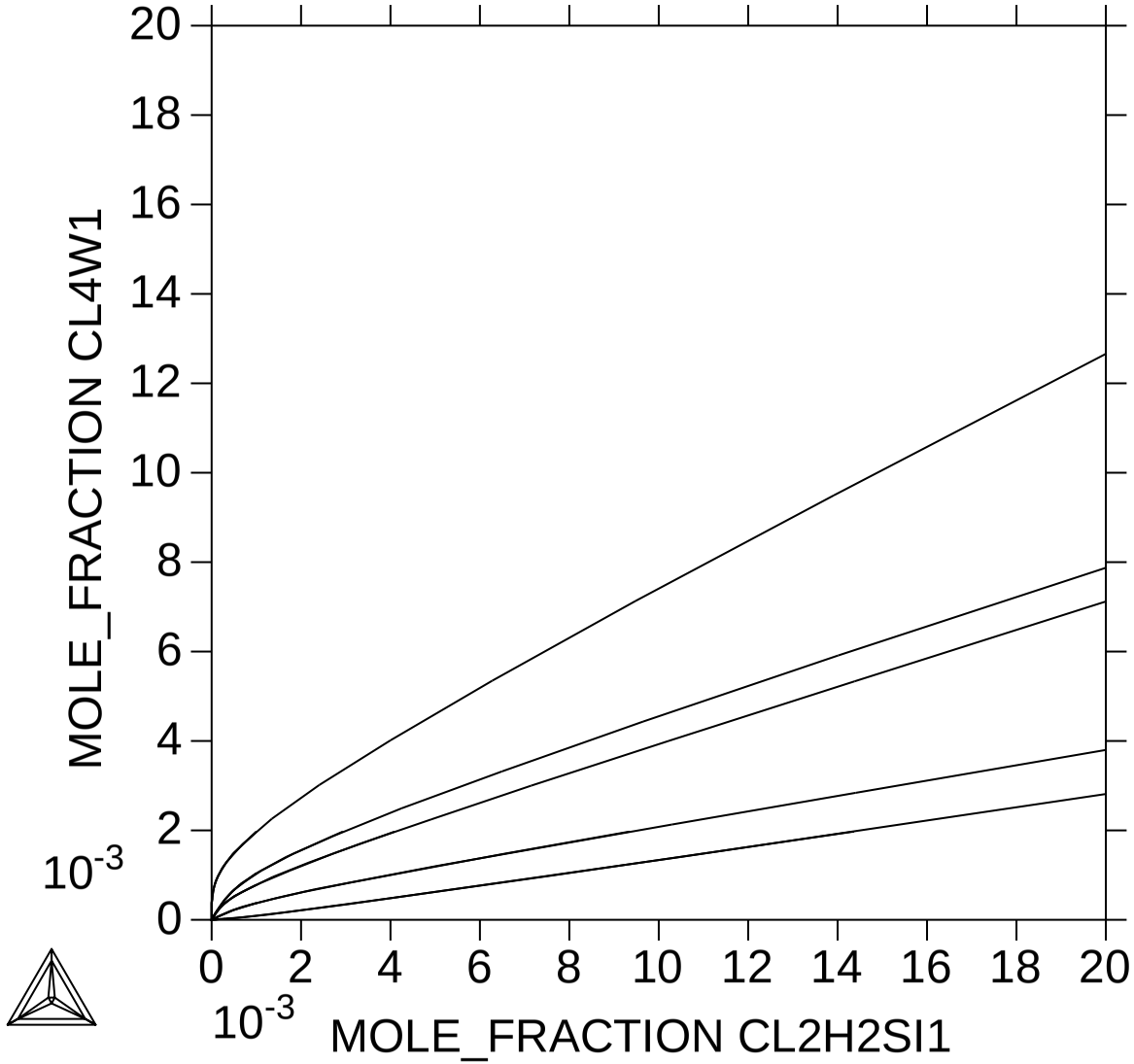
 Phase region boundary  23 at:   1.000E-03  7.855E-04
     GAS
  ** SI2W1_S
     SI3W5_S
 Calculated..            6  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: tcex27.POLY3
 CPU time for mapping          50  seconds
POLY_3: @@
POLY_3: @@ Plot the diagram in the post processor
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

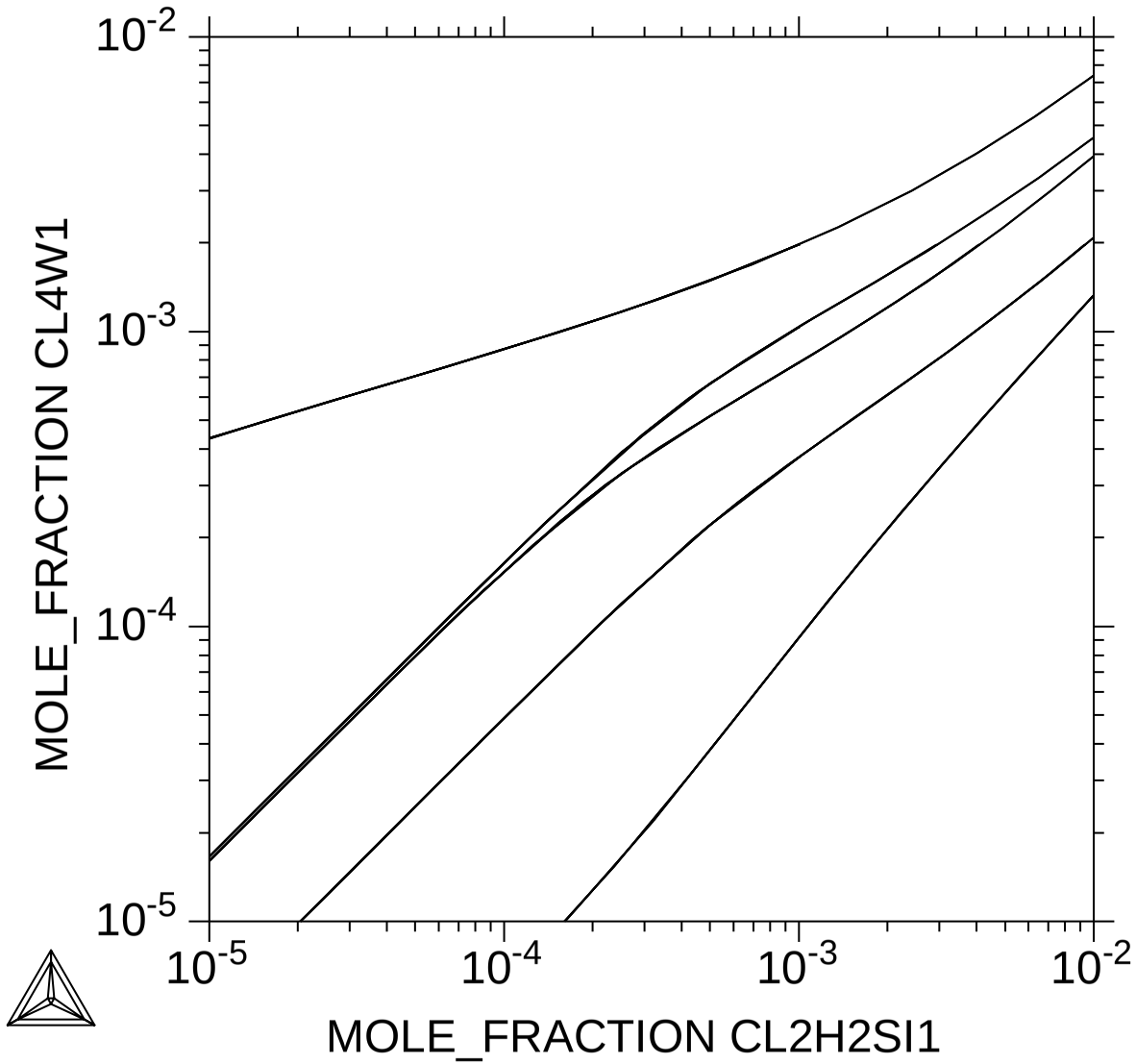
POST:
POST: set-title example 27a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Better with logarithmic axis
POST: s-a-ty x log
   ... the command in full is SET_AXIS_TYPE
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-s x n 1e-5 .01
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 1e-5 .01
   ... the command in full is SET_SCALING_STATUS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
```

POST: *@@*
POST: **set-title example 27b**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@Identify one of the phase regions***
POST: **add .0005 2e-5**
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in 0 s
 Calculated POLY solution 0 s, total time 0 s
 Stable phases are: GAS+SI2W1_S+SI_S
Text size: /.3999999762/:
POST: **set-title example 27c**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **set-inter**
... the command in full is SET_INTERACTIVE_MODE
POST: CPU time 53 seconds

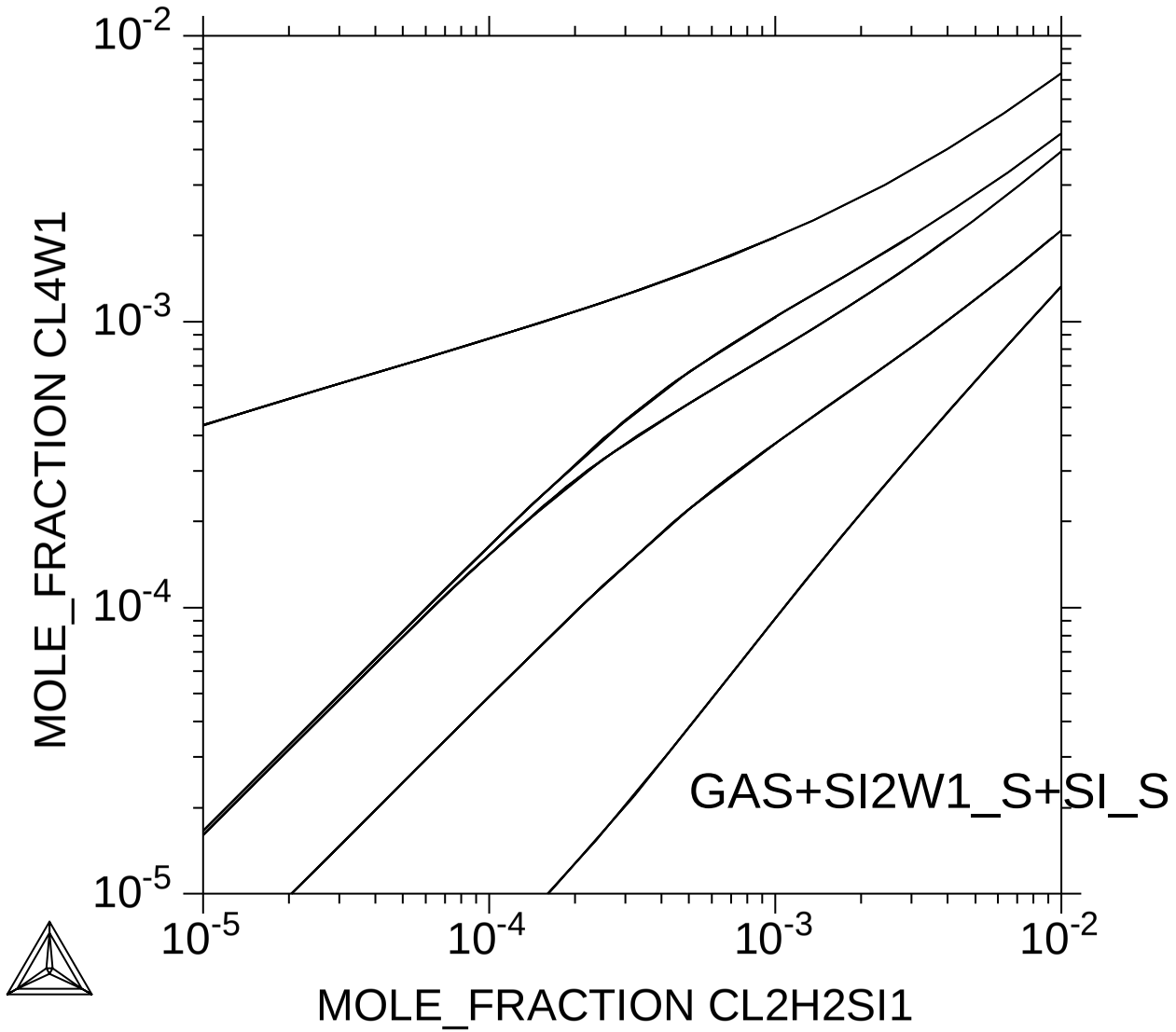
THERMO-CALC (2009.04.15:03.06) :example 27a
DATABASE:SSUB4
N=1., X(AR)=0.9, X(CL1H1)=1.35032E-15, T=1000, P=1.01325E5;



THERMO-CALC (2009.04.15:03.06) :example 27b
DATABASE:SSUB4
N=1., X(AR)=0.9, X(CL1H1)=1.35032E-15, T=1000, P=1.01325E5;



THERMO-CALC (2009.04.15:03.06) :example 27c
DATABASE:SSUB4
N=1., X(AR)=0.9, X(CL1H1)=1.35032E-15, T=1000, P=1.01325E5;



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Calculation of PRE

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example showing calculation of PRE (Pitting Resistance Equivalence)
SYS: @@ for a duplex stainless steel
SYS: @@
SYS: set-log ex28,,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ set the nominal composition
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/:  tcfe6
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: cr 25 ni 7 mo 4 c .002 n .27 si .3 mn .3
Next alloying element:
Temperature (C) /1000/:  1050
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MO  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 N  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED

 This database has following phases for the defined system

 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M6C                     M5C2
 M3C2                    MC_ETA                  MC_SHP
 KSI_CARBIDE             A1_KAPPA                KAPPA
 Z_PHASE                 FE4N_LP1                FECN_CHI
 PI                      SIGMA                   MU_PHASE
 P_PHASE                 R_PHASE                 CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   NI3TI                   AL4C3
 FE8SI2C                 SIC

Reject phase(s) /NONE/:  *
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
```

```
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M6C                     M5C2
 M3C2                    MC_ETA                  MC_SHP
 KSI_CARBIDE             A1_KAPPA                KAPPA
 Z_PHASE                 FE4N_LP1                FECN_CHI
 PI                      SIGMA                   MU_PHASE
 P_PHASE                 R_PHASE                 CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   NI3TI                   AL4C3
 FE8SI2C                 SIC  REJECTED
Restore phase(s):: fcc bcc hcp m23 sigma
 FCC_A1                  BCC_A2                  HCP_A3
 M23C6                   SIGMA  RESTORED
Restore phase(s): /NONE/:

 ..................................................

    The following phases are retained in this system:

 BCC_A2                   FCC_A1                   HCP_A3
 M23C6                    SIGMA

 ..................................................

OK? /Y/:
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'K. Frisk, TRITA-MAC 393 (1989); CR-N, FE-N, MO-N, CR-MO-N'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
                    :
                    :
                    :
  'Unassessed parameter'
  'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'C. Qiu, Metall. Trans. A, 24A (1993), 2393-2409; Cr-Fe-Mn-N'
  'P. Villars and L.D. Calvert (1985). Pearson´s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
 Calculated        11328  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Creating a new composition set SIGMA#2
 Creating a new composition set SIGMA#3
 Calculated POLY solution       2 s, total time     2  s
POLY_3:
POLY_3:
POLY_3: save tcex28 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/: VWCS
```

```
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=1323.15, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
    W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1323.15 K (  1050.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -7.36372E+04,  Enthalpy  3.91632E+04,  Volume  7.43499E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 2.8934E-05 -1.1497E+05 SER
 CR                      2.6597E-01  2.5000E-01 2.5102E-03 -6.5869E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.6011E-03 -7.0817E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.6138E-06 -1.4142E+05 SER
 MO                      2.3064E-02  4.0000E-02 6.3441E-04 -8.1001E+04 SER
 N                       1.0663E-02  2.7000E-03 4.5323E-07 -1.6070E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.2113E-04 -9.9217E+04 SER
 SI                      5.9088E-03  3.0000E-03 3.2519E-09 -2.1501E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 5.5763E-01, Mass 3.0640E+01, Volume fraction 5.5307E-01  Mass fractions:
 FE  6.36999E-01  NI  8.57940E-02  N   4.60149E-03  SI  2.58552E-03
 CR  2.34729E-01  MO  3.18218E-02  MN  3.43771E-03  C   3.18713E-05

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.4237E-01, Mass 2.4678E+01, Volume fraction 4.4693E-01  Mass fractions:
 FE  6.24180E-01  NI  5.03909E-02  SI  3.51459E-03  N   3.39204E-04
 CR  2.68960E-01  MO  5.01537E-02  MN  2.45656E-03  C   5.26115E-06
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Calculate the temperature for equal amount
POLY_3: c-s p bcc=fix .5
   ... the command in full is CHANGE_STATUS
POLY_3: s-c t=none
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated        11328  grid points in           0  s
    11 ITS,  CPU TIME USED   1 SECONDS
POLY_3: sh t
   ... the command in full is SHOW_VALUE
 T=1381.4276
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3, W(SI)=3E-3,
    W(MN)=3E-3, P=1E5, N=1
 FIXED PHASES
 BCC_A2=.5
 DEGREES OF FREEDOM 0

 Temperature   1381.43 K (  1108.28 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -7.86534E+04,  Enthalpy  4.13847E+04,  Volume  7.46323E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 2.7951E-05 -1.2043E+05 SER
 CR                      2.6597E-01  2.5000E-01 2.0954E-03 -7.0845E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.3658E-03 -7.5761E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.3755E-06 -1.4875E+05 SER
 MO                      2.3064E-02  4.0000E-02 4.7945E-04 -8.7785E+04 SER
 N                       1.0663E-02  2.7000E-03 6.6471E-07 -1.6337E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.0967E-04 -1.0473E+05 SER
 SI                      5.9088E-03  3.0000E-03 4.7824E-09 -2.2005E+05 SER

 BCC_A2                      Status FIXED       Driving force  0.0000E+00
 Moles 5.0095E-01, Mass 2.7933E+01, Volume fraction 5.0554E-01  Mass fractions:
 FE  6.26660E-01  NI  5.38048E-02  SI  3.46210E-03  N   4.70180E-04
```

```
 CR  2.64435E-01  MO  4.86102E-02  MN  2.55179E-03  C   5.96269E-06

 FCC_A1#1                  Status ENTERED     Driving force  0.0000E+00
 Moles 4.9905E-01, Mass 2.7385E+01, Volume fraction 4.9446E-01  Mass fractions:
 FE  6.35993E-01  NI  8.65195E-02  N   4.97447E-03  SI  2.52865E-03
 CR  2.35276E-01  MO  3.12173E-02  MN  3.45719E-03  C   3.43184E-05
POLY_3: @@ enter the PRE functions
POLY_3: ent fun prefcc
   ... the command in full is ENTER_SYMBOL
Function: 100*w(fcc,cr)+300*w(fcc,mo)+1600*w(fcc,n);
POLY_3: ent fun prebcc
   ... the command in full is ENTER_SYMBOL
Function: 100*w(bcc,cr)+300*w(bcc,mo)+1600*w(bcc,n);
POLY_3: l-sy
   ... the command in full is LIST_SYMBOLS
 DEFINED FUNCTIONS AND VARIABLES%
    PREFCC=100*W(FCC_A1#1,CR)+300*W(FCC_A1#1,MO)+1600*W(FCC_A1#1,N)
    PREBCC=100*W(BCC_A2,CR)+300*W(BCC_A2,MO)+1600*W(BCC_A2,N)
POLY_3: eval
   ... the command in full is EVALUATE_FUNCTIONS
Name(s): *
 PREFCC=40.851953
 PREBCC=41.778859
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Now vary the nitrogen content
POLY_3: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/:  w(n)
Min value /0/:  .001
Max value /1/:  .005
Increment /1E-04/:  1E-04
POLY_3: li-ax
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(N)                Min: 1E-3      Max: 5E-3      Inc: 1E-4
POLY_3: save tcex28 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  NORMAL
 No initial equilibrium, using default
 Step will start from axis value   0.270000E-02
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from   0.270000E-02 for:
     BCC_A2
     FCC_A1#1
 Global test at  3.50000E-03 .... OK
 Global test at  4.50000E-03 .... OK
 Terminating at   0.500000E-02
 Calculated    26 equilibria

 Phase Region from   0.270000E-02 for:
     BCC_A2
     FCC_A1#1
 Global test at  1.90000E-03 .... OK
 Global check of adding phase at  1.88244E-03
 Calculated    11 equilibria

 Phase Region from   0.188244E-02 for:
     BCC_A2
     FCC_A1#1
     SIGMA#1
 Global test at  1.80000E-03 .... OK
 Global test at  1.60000E-03 .... OK
 Global test at  1.10000E-03 .... OK
 Terminating at   0.100000E-02
 Calculated    12 equilibria
 *** Buffer saved on file: tcex28.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST:
```

```
POST: @@ first plot how the temperature varies
POST: s-d-a x w(n)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 28a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ then plot the PRE
POST: ent tab pp
   ... the command in full is ENTER_SYMBOL
Variable(s): prefcc prebcc
&
POST:
POST: s-d-a y pp
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 28b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ add the temperature as tic marks
POST: s-d-a z t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 800 1300
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 28c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: back
POLY_3: @@ check how close we are to form Cr2N
POLY_3: read tcex28
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: @@ Restore BCC as entered
POLY_3: c-s p bcc=ent 1
   ... the command in full is CHANGE_STATUS
POLY_3: s-c t=1323
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        11328  grid points in            1  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     2  s
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
    W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1323.00 K (  1049.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -7.36244E+04,  Enthalpy  3.91576E+04,  Volume  7.43492E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 2.8937E-05 -1.1496E+05 SER
 CR                      2.6597E-01  2.5000E-01 2.5114E-03 -6.5857E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.6017E-03 -7.0804E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.6144E-06 -1.4140E+05 SER
 MO                      2.3064E-02  4.0000E-02 6.3488E-04 -8.0984E+04 SER
```

```
 N                      1.0663E-02  2.7000E-03 4.5278E-07 -1.6069E+05 SER
 NI                     6.5978E-02  7.0000E-02 1.2117E-04 -9.9203E+04 SER
 SI                     5.9088E-03  3.0000E-03 3.2485E-09 -2.1500E+05 SER

 FCC_A1#1                   Status ENTERED     Driving force  0.0000E+00
 Moles 5.5777E-01, Mass 3.0647E+01, Volume fraction 5.5321E-01  Mass fractions:
 FE  6.37001E-01  NI  8.57922E-02  N   4.60067E-03  SI  2.58565E-03
 CR  2.34728E-01  MO  3.18233E-02  MN  3.43767E-03  C   3.18660E-05

 BCC_A2                     Status ENTERED     Driving force  0.0000E+00
 Moles 4.4223E-01, Mass 2.4671E+01, Volume fraction 4.4679E-01  Mass fractions:
 FE  6.24173E-01  NI  5.03822E-02  SI  3.51472E-03  N   3.38915E-04
 CR  2.68972E-01  MO  5.01574E-02  MN  2.45631E-03  C   5.25959E-06
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Find out at which temperature sigma will form
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: sigma
 You must release one of these conditions
 T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
 W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/:  t
 Testing POLY result by global minimization procedure
 Calculated        11328  grid points in           1  s
To form SIGMA the condition is set to T=1292.91904984
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Find temperature for Cr2N, set start constitution first to
POLY_3: @@ make sure hcp#2 is nitride
POLY_3: s-s-c hcp#2 *
   ... the command in full is SET_START_CONSTITUTION
POLY_3: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: hcp#2
 You must release one of these conditions
 T=1292.92, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
 W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/:  t
 Testing POLY result by global minimization procedure
 Calculated        11328  grid points in           0  s
To form HCP the condition is set to T=1259.27248483
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=1259.27, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
    W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1259.27 K (   986.12 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -6.82552E+04,  Enthalpy  3.63967E+04,  Volume  7.38090E-06

 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 C                      9.2112E-05  2.0000E-05 2.9964E-05 -1.0905E+05 SER
 CR                     2.6597E-01  2.5000E-01 3.0773E-03 -6.0557E+04 SER
 FE                     6.2530E-01  6.3128E-01 1.9346E-03 -6.5416E+04 SER
 MN                     3.0208E-03  3.0000E-03 2.8836E-06 -1.3356E+05 SER
 MO                     2.3064E-02  4.0000E-02 7.3164E-04 -7.5597E+04 SER
 N                      1.0663E-02  2.7000E-03 2.8053E-07 -1.5796E+05 SER
 NI                     6.5978E-02  7.0000E-02 1.3184E-04 -9.3540E+04 SER
 SI                     5.9088E-03  3.0000E-03 2.2874E-09 -2.0831E+05 SER

 FCC_A1#1                   Status ENTERED     Driving force  0.0000E+00
 Moles 6.8920E-01, Mass 3.7855E+01, Volume fraction 6.8587E-01  Mass fractions:
 FE  6.48029E-01  NI  8.31667E-02  N   3.87086E-03  SI  3.08632E-03
 CR  2.31778E-01  MO  2.66514E-02  MN  3.39040E-03  C   2.78089E-05

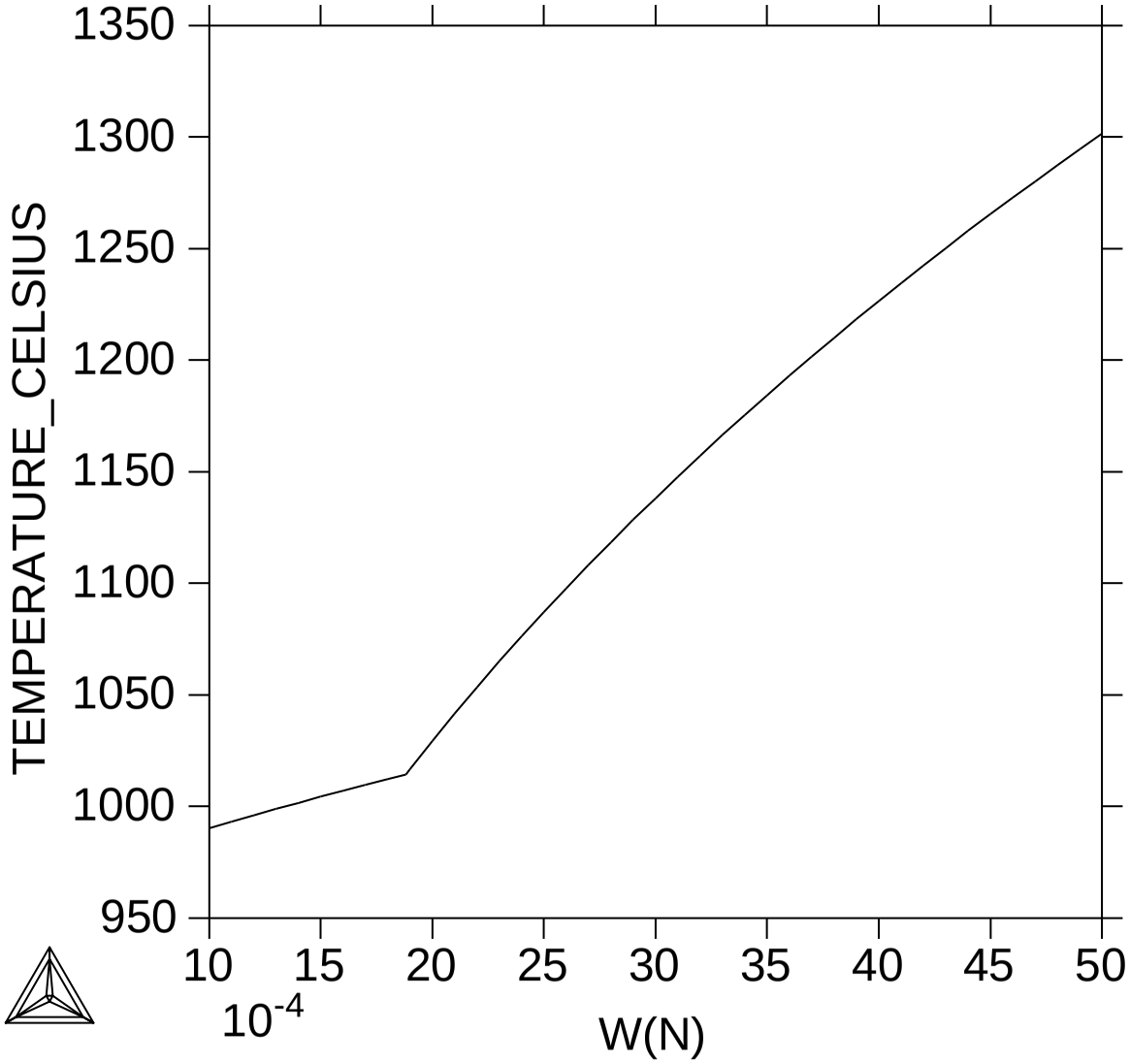
 BCC_A2                     Status ENTERED     Driving force  0.0000E+00
 Moles 2.1649E-01, Mass 1.2027E+01, Volume fraction 2.1925E-01  Mass fractions:
```

```
 FE  6.29278E-01  NI  4.56640E-02  SI  4.06079E-03  N   2.35187E-04
 CR  2.76015E-01  MO  4.23998E-02  MN  2.34302E-03  C   4.46220E-06

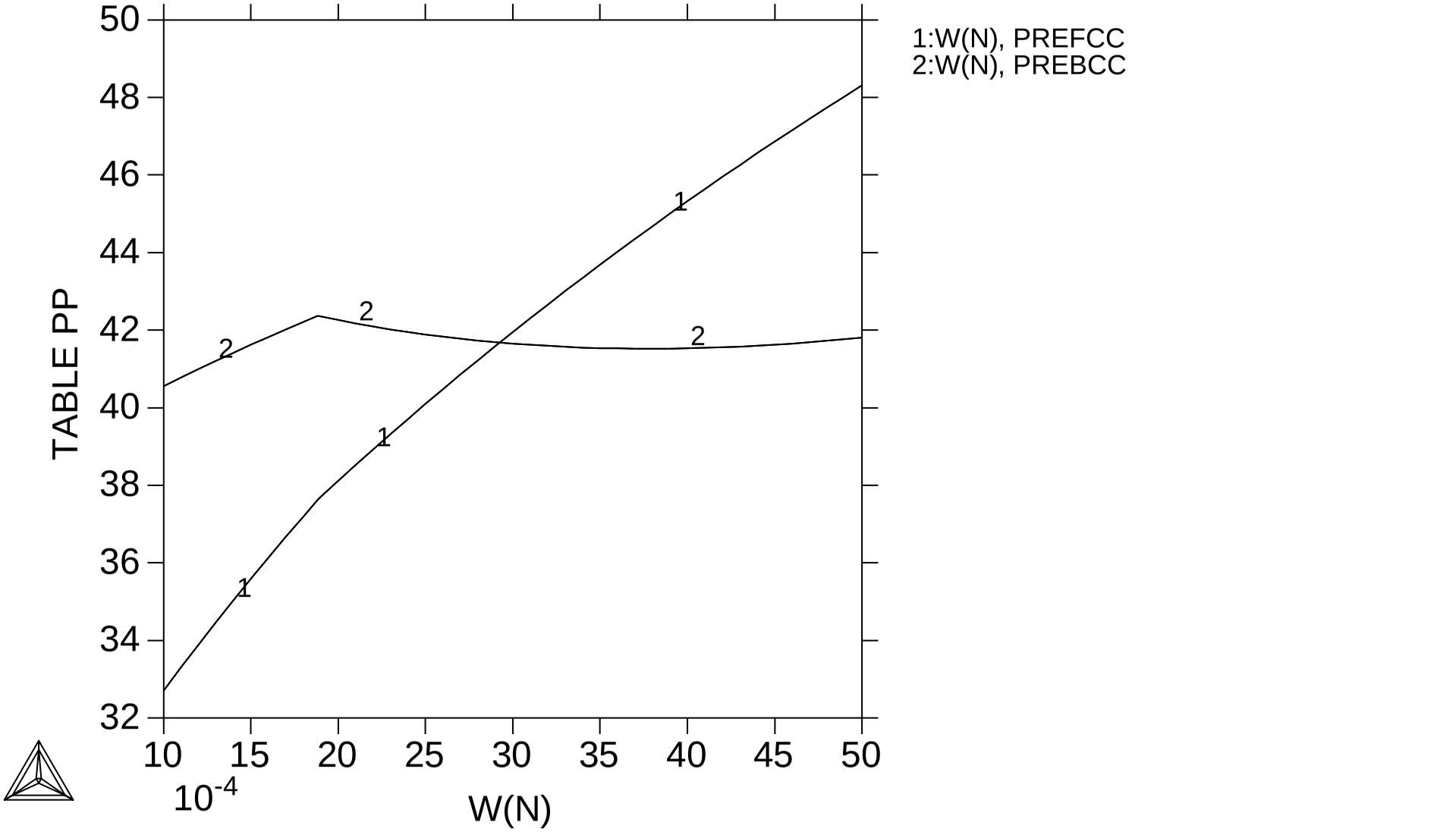
 SIGMA#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.4318E-02, Mass 5.4368E+00, Volume fraction 9.4879E-02  Mass fractions:
 FE  5.19091E-01  MO  1.27634E-01  MN  1.73510E-03  C   0.00000E+00
 CR  3.19330E-01  NI  3.21573E-02  SI  5.24586E-05  N   0.00000E+00

 HCP_A3#2                   Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CR  8.21501E-01  MO  4.07568E-02  NI  1.38869E-03  C   2.54908E-04
 N   1.07833E-01  FE  2.76173E-02  MN  6.47751E-04  SI  2.24368E-08
POLY_3: @@ Rapid cooling needed to avoid these phases!
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3: CPU time          25  seconds
```

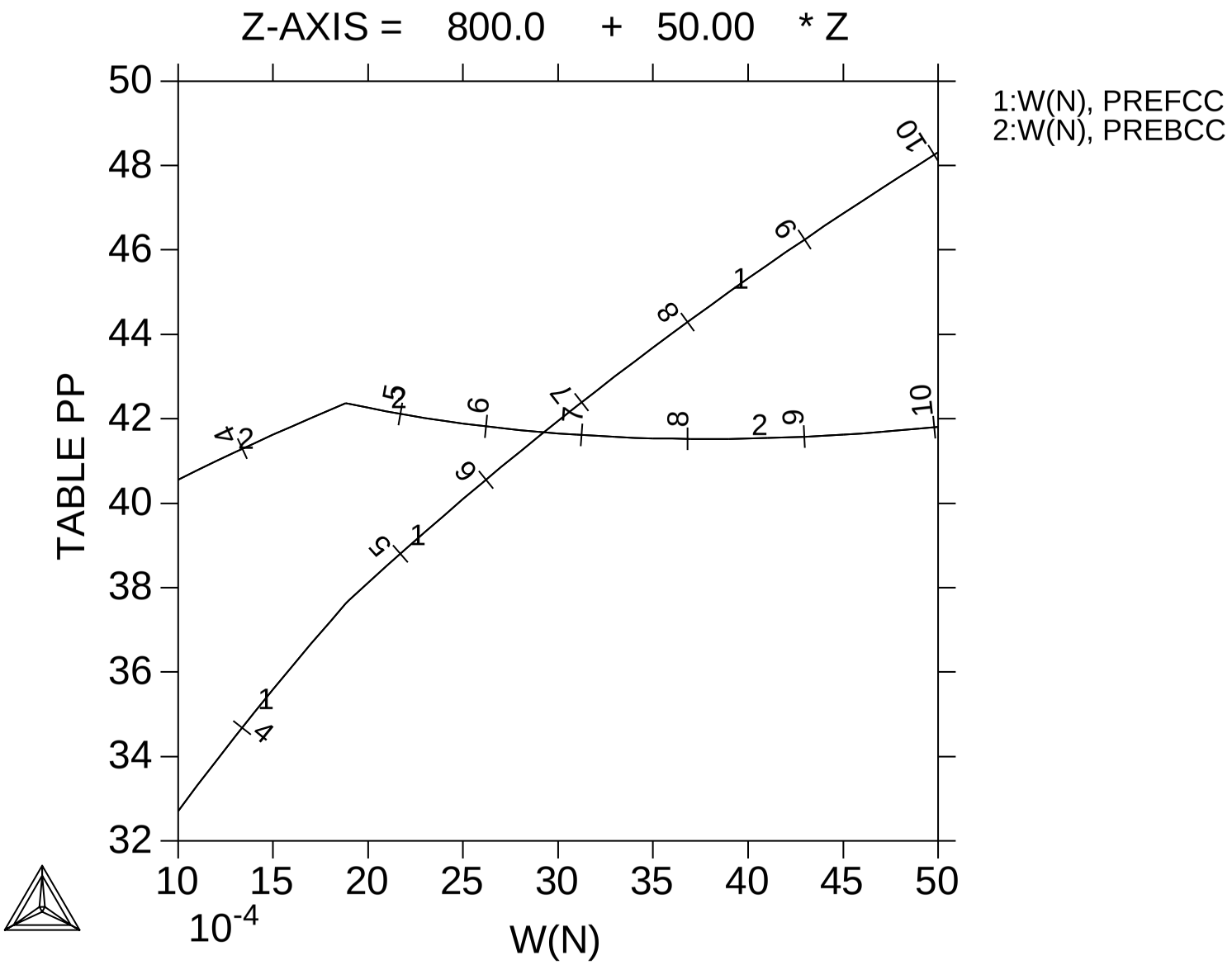
THERMO-CALC (2009.04.15:03.07) :example 28a
DATABASE:TCFE6
W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(SI)=3E-3, W(MN)=3E-3, P=1E5,
N=1. FIXED PHASES: BCC_A2=.5;



THERMO-CALC (2009.04.15:03.07) :example 28b
DATABASE:TCFE6
W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(SI)=3E-3, W(MN)=3E-3, P=1E5,
N=1. FIXED PHASES: BCC_A2=.5;



THERMO-CALC (2009.04.15:03.07) :example 28c
DATABASE:TCFE6



29

Calculation of speciation of a gas

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of speciation of a gas
SYS: @@
SYS: set-log ex29,,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw ssub4
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v4

 VA  DEFINED
TDB_SSUB4:
TDB_SSUB4: d-sys c o h s
   ... the command in full is DEFINE_SYSTEM
 C                       O                       H
 S  DEFINED
TDB_SSUB4: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 GAS:G       :C C2 C3 C4 C5 C60 C1H1 C1H1O1 C1H1O2 C1H2 C1H2O1 C1H2O2_CIS
  C1H2O2_DIOXIRANE C1H2O2_TRANS C1H3 C1H3O1_CH2OH C1H3O1_CH3O C1H4 C1H4O1
  C1O1 C1O1S1 C1O2 C1S1 C1S2 C2H1 C2H2 C2H2O1 C2H3 C2H4 C2H4O1_ACETALDEHYDE
  C2H4O1_OXIRANE C2H4O2_ACETICACID C2H4O2_DIOXETANE C2H4O3_123TRIOXOLANE
  C2H4O3_124TRIOXOLANE C2H5 C2H6 C2H6O1 C2H6O2 C2O1 C3H1 C3H4_1 C3H4_2 C3H6
  C3H6O1 C3H6_2 C3H8 C3O2 C4H10_1 C4H10_2 C4H1 C4H2 C4H4_1_3 C4H4 C4H6_1
  C4H6_2 C4H6_3 C4H6_4 C4H6_5 C4H8 C4H8_1 C4H8_2 C4H8_3 C4H8_4 C4H8_5 C6H6
  C6H6O1 H H2 H1O1 H1O1S1_HSO H1O1S1_SOH H1O2 H1S1 H2O1 H2O1S1_H2SO
  H2O1S1_HSOH H2O2 H2O4S1 H2S1 H2S2 O2 O3 O O1S1 O1S2 O2S1 O3S1 S S2 S3 S4
  S5 S6 S7 S8:
 C_S         :C:
 C_L         :C:
 DIAMOND     :C:
 C1H2O2_L    :C1H2O2:
 C1H4O1_L    :C1H4O1:
 C1S2_L      :C1S2:
 C2H4O2_L    :C2H4O2:
 C2H6O1_L    :C2H6O1:
 C2H6O2_L    :C2H6O2:
 C60_S       :C60:
 C6H6_L      :C6H6:
 H10O8S1_L   :H10O8S1:
 H15O10_5S1_L :H15O10.5S1:
 H2O1_L      :H2O1:
 H2O2_L      :H2O2:
 H2O4S1_L    :H2O4S1:
 H4O5S1_L    :H4O5S1:
 H6O6S1_L    :H6O6S1:
 H8O7S1_L    :H8O7S1:
 S_S         :S:
 S_S2        :S:
 S_L         :S:
TDB_SSUB4: @?<Hit_return_to_continue>
TDB_SSUB4: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
```

```
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
   C1H1<G> T.C.R.A.S. Class: 2
   C1H1O1<G> T.C.R.A.S. Class: 4
      FORMYL <GAS>
   C1H1O2<G> T.C.R.A.S. Class: 6
   C1H2<G> T.C.R.A.S. Class: 5
      METHYLENE <GAS>
                  :
                  :
                  :
   H6O6S1 THERMODATA 01/93
      H2SO4-2H2O
      28/01/93
   H8O7S1 Janaf 4th. Edition
      SULFURIC ACID TRIHYDRATE
   S1 T.C.R.A.S Class: 5
      Data provided by T.C.R.A.S. October 1994.
      Data refitted by I.A.
 -OK-
TDB_SSUB4: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT              STATUS    REF. STATE     T(K)           P(Pa)
 VA                     ENTERED   SER
 C                      ENTERED   SER
 H                      ENTERED   SER
 O                      ENTERED   SER
 S                      ENTERED   SER
POLY_3: s-i-a n(h2)=10
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(H)=20
 DEGREES OF FREEDOM 5
POLY_3: s-i-a n(c1o2)=5
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-i-a n(o2s1)=0.1
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1
 DEGREES OF FREEDOM 2
POLY_3: s-c t=1000 p=1e5
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          118  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB4

 Conditions:
 N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1, T=1000, P=1E5
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  3.53000E+01,  Mass in grams  2.46609E+02
 Total Gibbs energy -4.82824E+06,  Enthalpy -1.54921E+06,  Volume  1.23971E+00

 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 C                      5.0000E+00  2.4352E-01 3.4847E-02 -2.7910E+04 SER
```

```
 H                      2.0000E+01  8.1741E-02 1.0525E-04 -7.6154E+04 SER
 O                      1.0200E+01  6.6173E-01 7.2141E-17 -3.0903E+05 SER
 S                      1.0000E-01  1.3003E-02 9.1466E-08 -1.3476E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 3.5300E+01, Mass 2.4661E+02, Volume fraction 1.0000E+00  Mass fractions:
 O  6.61734E-01  C  2.43523E-01  H  8.17406E-02  S  1.30027E-02
 Constitution:
 H2           4.42736E-01  C3H6_2       1.11399E-13  C4H6_3       6.48690E-21
 H2O1         2.15350E-01  C3H6         1.10240E-13  C4H4         3.35580E-21
 C1O1         1.95778E-01  H1O1S1_SOH   3.35036E-14  O2           1.79255E-21
 C1O2         1.36417E-01  C2H6O1       2.98678E-14  C2O1         1.66878E-21
 H2S1         6.57218E-03  C2H5         2.60816E-14  S5           8.95084E-22
 C1H4         3.01187E-03  C3H8         1.55219E-14  C2H2O1       5.16353E-22
 C1O1S1       1.34465E-04  C1H3O1_CH2OH 7.69302E-15  C4H6_5       3.26857E-22
 H1S1         5.08063E-08  H2O1S1_H2SO  2.59570E-15  C4H2         1.36450E-22
 C1H2O1       4.89873E-08  C3H6O1       1.36487E-15  C4H8         8.64311E-23
 C1H2O2_CIS   4.46604E-08  C2H3         1.30277E-15  C4H8_4       5.30112E-23
 H2S2         3.75745E-08  C3H4_2       1.28184E-15  H2O4S1       1.59729E-23
 C1S2         1.41821E-08  C3O2         7.11139E-16  C6H6O1       6.55562E-24
 S2           1.10500E-08  C3H4_1       3.44164E-16  H1O2         1.72311E-24
 C1H2O2_TRANS 6.42811E-09  H1O1S1_HSO   1.08974E-16  C2H1         3.18714E-25
 C2H6         3.64609E-09  C1H3O1_CH3O  1.80849E-17  S6           2.65463E-26
 C2H4         3.02667E-09  C2H4O1_OXIRA 2.11511E-18  C1H1         5.08634E-27
 H            1.51148E-09  C4H6_2       1.29360E-18  C4H4_1_3     4.75003E-27
 C1H4O1       1.14083E-09  S4           1.12104E-18  C3H1         9.91558E-28
 O2S1         2.26895E-10  C4H8_5       7.77387E-19  C1H2O2_DIOXI 4.40433E-30
 C1H3         1.88514E-10  C4H8_3       4.90029E-19  C            1.00000E-30
 H2O1S1_HSOH  8.67082E-11  C4H8_1       3.93895E-19  C2           1.00000E-30
 C2H4O1_ACETA 2.61120E-11  C4H8_2       3.45603E-19  C2H4O2_DIOXE 1.00000E-30
 C2H2         1.43254E-11  C2H6O2       2.59417E-19  C2H4O3_123TR 1.00000E-30
 O1S1         1.05406E-11  C1H2         2.13894E-19  C2H4O3_124TR 1.00000E-30
 C1H1O1       9.19785E-12  C4H10_1      8.31953E-20  C3           1.00000E-30
 C1S1         5.40802E-12  C4H10_2      4.22679E-20  C4           1.00000E-30
 C2H4O2_ACETI 4.53120E-12  C6H6         3.95182E-20  C4H1         1.00000E-30
 H1O1         1.61961E-12  H2O2         2.47048E-20  C5           1.00000E-30
 O1S2         9.69426E-13  C4H6_4       1.91129E-20  C60          1.00000E-30
 C1H1O2       9.05180E-13  O3S1         1.73550E-20  O3           1.00000E-30
 S            7.19264E-13  C4H6_1       1.14077E-20  S7           1.00000E-30
 S3           1.46179E-13  O            6.65785E-21  S8           1.00000E-30
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-a-v 1 t 500 2000 50
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex29 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    1000.00
 Global calculation of initial equilibrium ....OK

 Phase Region from    1000.00     for:
     GAS
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
 Global test at  1.28000E+03 .... OK
 Global test at  1.38000E+03 .... OK
 Global test at  1.48000E+03 .... OK
 Global test at  1.58000E+03 .... OK
 Global test at  1.68000E+03 .... OK
 Global test at  1.78000E+03 .... OK
 Global test at  1.88000E+03 .... OK
 Global test at  1.98000E+03 .... OK
 Terminating at    2000.00
 Calculated   103 equilibria

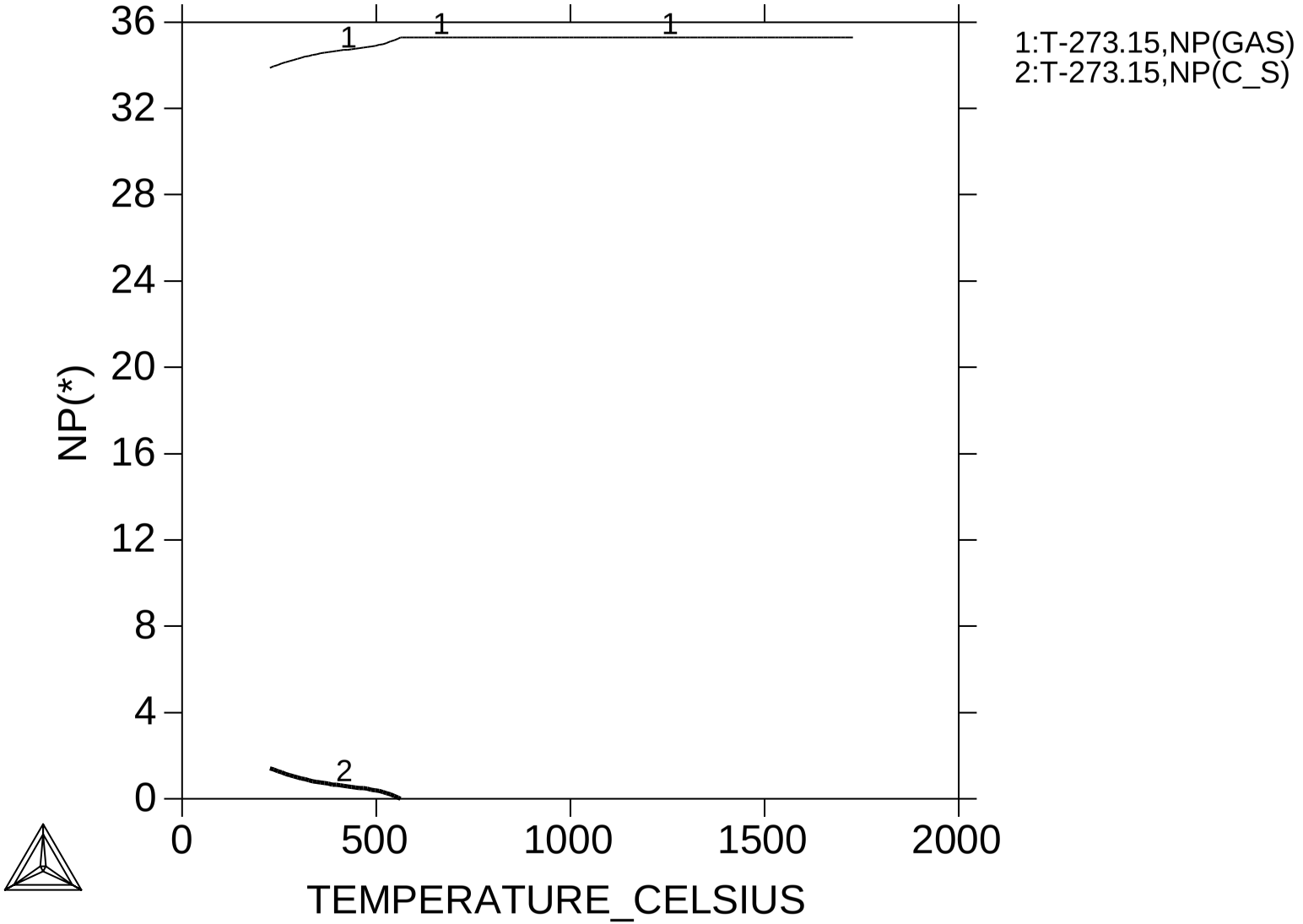
 Phase Region from    1000.00     for:
     GAS
 Global test at  9.20000E+02 .... OK
 Global check of adding phase at  8.35809E+02
 Calculated    19 equilibria
```

```
 Phase Region from    835.809     for:
     GAS
     C_S
 Global test at  7.60000E+02 .... OK
 Global test at  6.60000E+02 .... OK
 Global test at  5.60000E+02 .... OK
 Terminating at    500.000
 Calculated    37 equilibria
 *** Buffer saved on file: tcex29.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

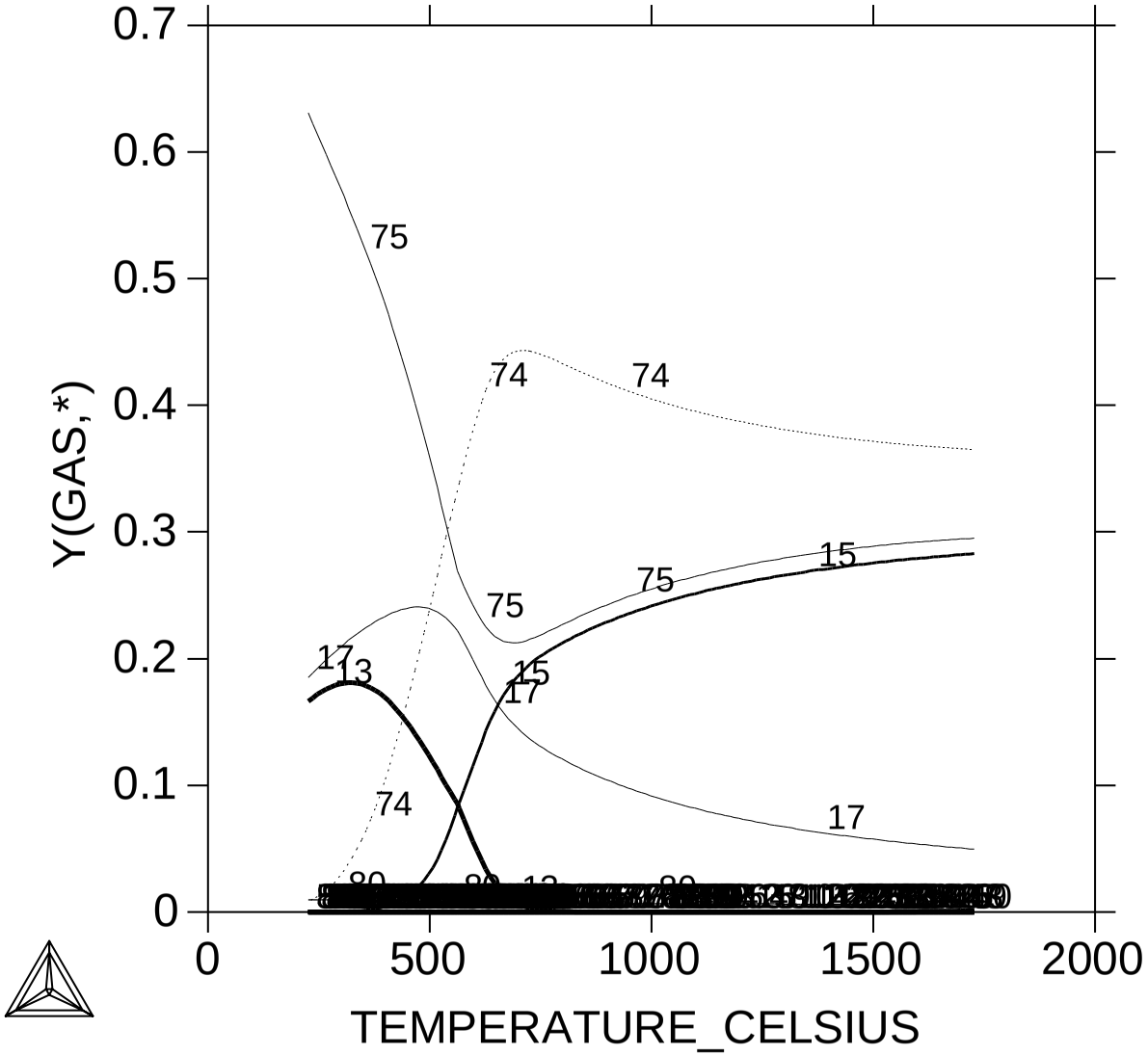
 Setting automatic diagram axis

POST:
POST: @@ plot amount of phases, mainly gas!
POST: s-d-a x t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: s-l f
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 29a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ plot gas speciation. y(gas,*) are partial
POST: @@ pressures expressed in bar (as total pressure
POST: @@ is one bar!). Set labels on the lines.
POST: s-d-a y y(gas,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 29b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Set logarithmic axis
POST: s-ax-ty
   ... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : y
AXIS TYPE /LINEAR/:  log
POST:
POST: @@ also set font size smaller to display more labels
POST: set-font
 CURRENT FONT: Cartographic Roman
SELECT FONTNUMBER /1/:
 NEW FONT: Cartographic Roman
FONT SIZE /.3400000036/:  .25
POST: set-title example 29c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Set scaling
POST: s-s y n 1e-12 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 29d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           4  seconds
```

THERMO-CALC (2009.04.15:03.07) :example 29a
DATABASE:SSUB4
N(H)=20., N(C)=5., N(O)=10.2, N(S)=0.1, P=1E5;

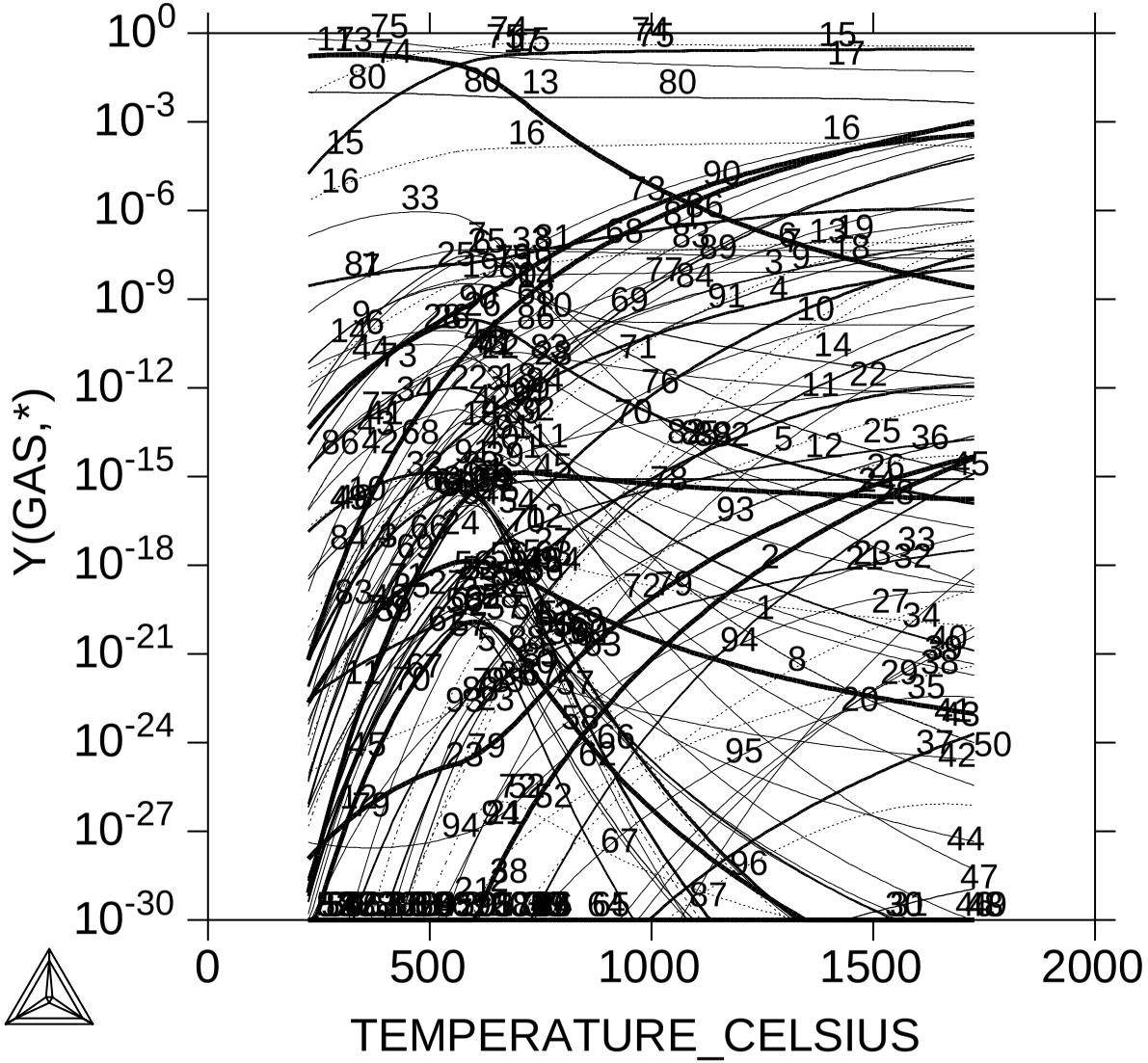


THERMO-CALC (2009.04.15:03.07) :example 29b
DATABASE:SSUB4
N(H)=20., N(C)=5., N(O)=10.2, N(S)=0.1, P=1E5;



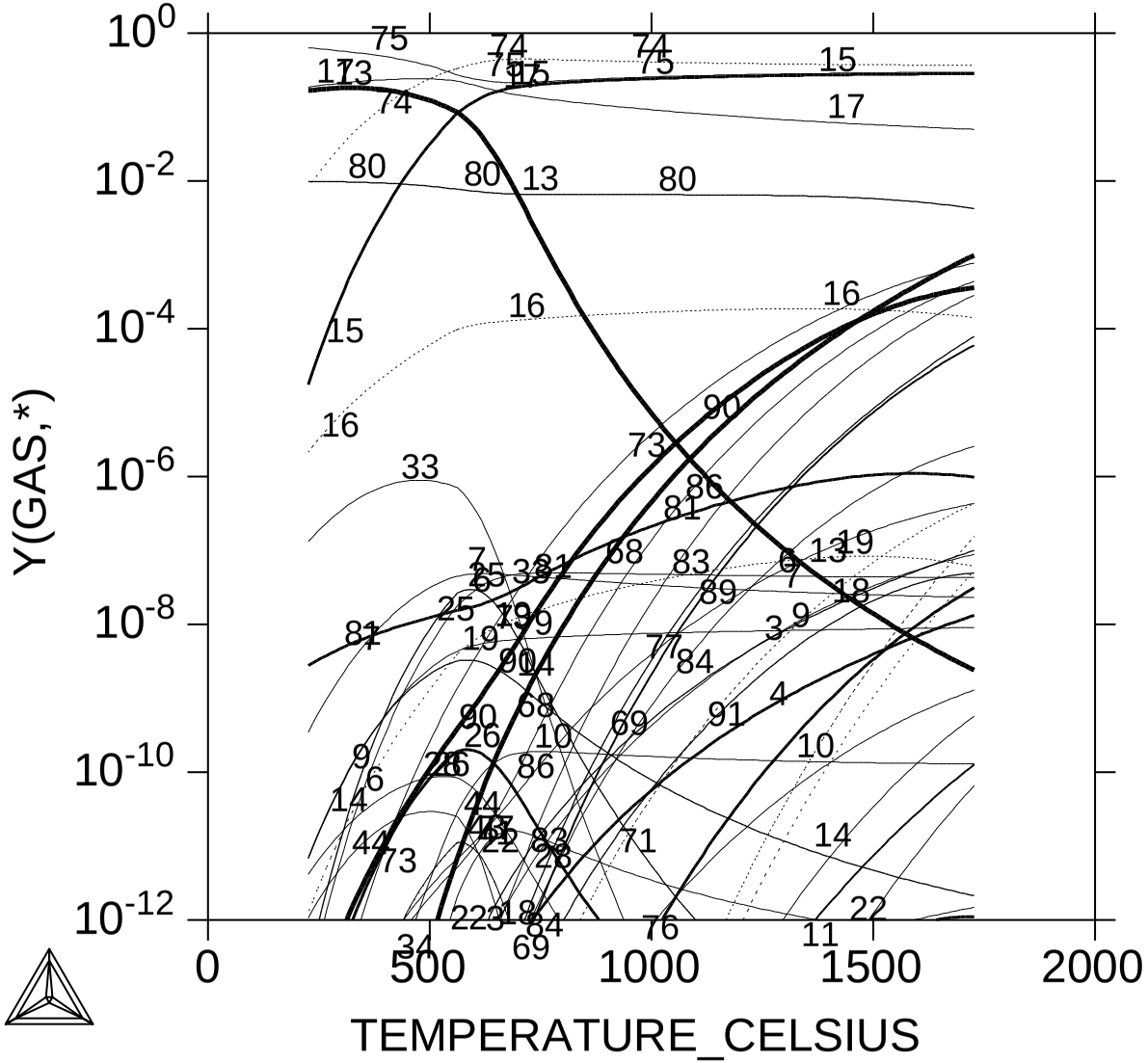
1:T-273.15,Y(GAS,C)
2:T-273.15,Y(GAS,C1H1)
3:T-273.15,Y(GAS,C1H1O1)
4:T-273.15,Y(GAS,C1H1O2)
5:T-273.15,Y(GAS,C1H2)
6:T-273.15,Y(GAS,C1H2O1)
7:T-273.15,Y(GAS,C1H2O2_CIS)
8:T-273.15,Y(GAS,C1H2O2_DIOXIRANE)
9:T-273.15,Y(GAS,C1H2O2_TRANS)
10:T-273.15,Y(GAS,C1H3)
11:T-273.15,Y(GAS,C1H3O1_CH2OH)
12:T-273.15,Y(GAS,C1H3O1_CH3O)
13:T-273.15,Y(GAS,C1H4)
14:T-273.15,Y(GAS,C1H4O1)
15:T-273.15,Y(GAS,C1O1)
16:T-273.15,Y(GAS,C1O1S1)
17:T-273.15,Y(GAS,C1O2)
18:T-273.15,Y(GAS,C1S1)
19:T-273.15,Y(GAS,C1S2)
20:T-273.15,Y(GAS,C2)
21:T-273.15,Y(GAS,C2H1)
22:T-273.15,Y(GAS,C2H2)
23:T-273.15,Y(GAS,C2H2O1)
24:T-273.15,Y(GAS,C2H3)
25:T-273.15,Y(GAS,C2H4)
26:T-273.15,Y(GAS,C2H4O1_ACETALDEHYDE)
27:T-273.15,Y(GAS,C2H4O1_OXIRANE)
28:T-273.15,Y(GAS,C2H4O2_ACETICACID)
29:T-273.15,Y(GAS,C2H4O2_DIOXETANE)
30:T-273.15,Y(GAS,C2H4O3_123TRIOXOLANE)
31:T-273.15,Y(GAS,C2H4O3_124TRIOXOLANE)
32:T-273.15,Y(GAS,C2H5)
33:T-273.15,Y(GAS,C2H6)
34:T-273.15,Y(GAS,C2H6O1)

THERMO-CALC (2009.04.15:03.07) :example 29c
DATABASE:SSUB4
N(H)=20., N(C)=5., N(O)=10.2, N(S)=0.1, P=1E5;



1:T-273.15,Y(GAS,C)
2:T-273.15,Y(GAS,C1H1)
3:T-273.15,Y(GAS,C1H1O1)
4:T-273.15,Y(GAS,C1H1O2)
5:T-273.15,Y(GAS,C1H2)
6:T-273.15,Y(GAS,C1H2O1)
7:T-273.15,Y(GAS,C1H2O2_CIS)
8:T-273.15,Y(GAS,C1H2O2_DIOXIRANE)
9:T-273.15,Y(GAS,C1H2O2_TRANS)
10:T-273.15,Y(GAS,C1H3)
11:T-273.15,Y(GAS,C1H3O1_CH2OH)
12:T-273.15,Y(GAS,C1H3O1_CH3O)
13:T-273.15,Y(GAS,C1H4)
14:T-273.15,Y(GAS,C1H4O1)
15:T-273.15,Y(GAS,C1O1)
16:T-273.15,Y(GAS,C1O1S1)
17:T-273.15,Y(GAS,C1O2)
18:T-273.15,Y(GAS,C1S1)
19:T-273.15,Y(GAS,C1S2)
20:T-273.15,Y(GAS,C2)
21:T-273.15,Y(GAS,C2H1)
22:T-273.15,Y(GAS,C2H2)
23:T-273.15,Y(GAS,C2H2O1)
24:T-273.15,Y(GAS,C2H3)
25:T-273.15,Y(GAS,C2H4)
26:T-273.15,Y(GAS,C2H4O1_ACETALDEHYDE)
27:T-273.15,Y(GAS,C2H4O1_OXIRANE)
28:T-273.15,Y(GAS,C2H4O2_ACETICACID)
29:T-273.15,Y(GAS,C2H4O2_DIOXETANE)
30:T-273.15,Y(GAS,C2H4O3_123TRIOXOLANE)
31:T-273.15,Y(GAS,C2H4O3_124TRIOXOLANE)
32:T-273.15,Y(GAS,C2H5)
33:T-273.15,Y(GAS,C2H6)
34:T-273.15,Y(GAS,C2H6O1)

THERMO-CALC (2009.04.15:03.07) :example 29d
DATABASE:SSUB4
N(H)=20., N(C)=5., N(O)=10.2, N(S)=0.1, P=1E5;



3:T-273.15,Y(GAS,C1H1O1)
4:T-273.15,Y(GAS,C1H1O2)
6:T-273.15,Y(GAS,C1H2O1)
7:T-273.15,Y(GAS,C1H2O2_CIS)
9:T-273.15,Y(GAS,C1H2O2_TRANS)
10:T-273.15,Y(GAS,C1H3)
11:T-273.15,Y(GAS,C1H3O1_CH2OH)
13:T-273.15,Y(GAS,C1H4)
14:T-273.15,Y(GAS,C1H4O1)
15:T-273.15,Y(GAS,C1O1)
16:T-273.15,Y(GAS,C1O1S1)
17:T-273.15,Y(GAS,C1O2)
18:T-273.15,Y(GAS,C1S1)
19:T-273.15,Y(GAS,C1S2)
22:T-273.15,Y(GAS,C2H2)
68:T-273.15,Y(GAS,H)
69:T-273.15,Y(GAS,H1O1)
71:T-273.15,Y(GAS,H1O1S1_SOH)
73:T-273.15,Y(GAS,H1S1)
74:T-273.15,Y(GAS,H2)
75:T-273.15,Y(GAS,H2O1)
76:T-273.15,Y(GAS,H2O1S1_H2SO)
77:T-273.15,Y(GAS,H2O1S1_HSOH)
80:T-273.15,Y(GAS,H2S1)
81:T-273.15,Y(GAS,H2S2)
83:T-273.15,Y(GAS,O1S1)
84:T-273.15,Y(GAS,O1S2)
86:T-273.15,Y(GAS,O2S1)
89:T-273.15,Y(GAS,S)
90:T-273.15,Y(GAS,S2)
91:T-273.15,Y(GAS,S3)
25:T-273.15,Y(GAS,C2H4)
26:T-273.15,Y(GAS,C2H4O1_ACETALDEHYDE)

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Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy

Part A. Step-by-step calculation

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example of Scheil calculation for Al-4Mg-2Si-2Cu
SYS: @@    Part A: step-by-step calculation
SYS: @@
SYS:
SYS: go d
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw u tcex30_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
TDB_USER: def-ele al cu mg si
 AL                      CU                      MG
 SI  DEFINED
TDB_USER: get
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 Reference REF1       missing
 Reference REF1       missing
 Reference REF1       missing
 Reference REF1       missing
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
 -OK-
TDB_USER: go p-3
 POLY version  3.32,  Dec 2007
POLY_3: s-c p=101325 n=1 t=1000 w(si)=0.02 w(mg)=0.04 w(cu)=0.02
POLY_3: c-e
 Using global minimization procedure
 Calculated        26470  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e,,
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 P=1.01325E5, N=1, T=1000, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.71965E+01
 Total Gibbs energy -4.56562E+04,  Enthalpy  3.06144E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      9.2731E-01  9.2000E-01 5.4982E-03 -4.3263E+04 SER
 CU                      8.5596E-03  2.0000E-02 5.9020E-07 -1.1925E+05 SER
 MG                      4.4759E-02  4.0000E-02 1.0064E-04 -7.6526E+04 SER
 SI                      1.9367E-02  2.0000E-02 1.1370E-03 -5.6367E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00  Mass fractions:
 AL  9.20000E-01  MG  4.00000E-02  SI  2.00000E-02  CU  2.00000E-02
```

```
POLY_3: @@ calculate liquidus temperature in order to choose
POLY_3: @@  a starting temperature where only liquid exists
POLY_3: c-st phase fcc_a1=fix 0
POLY_3: s-c t=none
POLY_3: c-e
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated        26470  grid points in           0  s
    12 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 P=1.01325E5, N=1, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
 FIXED PHASES
 FCC_A1=0
 DEGREES OF FREEDOM 0

 Temperature    897.74 K (   624.59 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.71965E+01
 Total Gibbs energy -3.80281E+04,  Enthalpy  2.73862E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      9.2731E-01  9.2000E-01 8.2190E-03 -3.5838E+04 SER
 CU                      8.5596E-03  2.0000E-02 5.5836E-07 -1.0747E+05 SER
 MG                      4.4759E-02  4.0000E-02 1.2754E-04 -6.6933E+04 SER
 SI                      1.9367E-02  2.0000E-02 2.2867E-03 -4.5388E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00  Mass fractions:
 AL  9.20000E-01  MG  4.00000E-02  CU  2.00000E-02  SI  2.00000E-02

 FCC_A1                      Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 AL  9.85194E-01  MG  1.12509E-02  CU  1.91685E-03  SI  1.63879E-03
POLY_3: show t
 T=897.74074
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-c t
Value /897.7407448/:  900
POLY_3: c-st phase
Phase name(s): fcc_a1
Status: /ENTERED/:  ENTERED
Start value, number of moles /0/:  0
POLY_3: c-e
 Using global minimization procedure
 Calculated        26470  grid points in           1  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: l-e,,
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 P=1.01325E5, N=1, T=900, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
 DEGREES OF FREEDOM 0

 Temperature    900.00 K (   626.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.71965E+01
 Total Gibbs energy -3.81928E+04,  Enthalpy  2.74567E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      9.2731E-01  9.2000E-01 8.1424E-03 -3.5998E+04 SER
 CU                      8.5596E-03  2.0000E-02 5.5930E-07 -1.0773E+05 SER
 MG                      4.4759E-02  4.0000E-02 1.2687E-04 -6.7141E+04 SER
 SI                      1.9367E-02  2.0000E-02 2.2488E-03 -4.5627E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00  Mass fractions:
 AL  9.20000E-01  MG  4.00000E-02  CU  2.00000E-02  SI  2.00000E-02
POLY_3: s-a-v 1 t
Min value /0/:  750 900 1
POLY_3:
```

```
POLY_3: ent var nl=1;
POLY_3: ent var nfcc=0;
POLY_3: ent var nl=np(liquid)*nl;
POLY_3: ent fun ns=1-nl;
POLY_3: ent var nfcc=nfcc+nl*np(fcc_a1);
POLY_3: ent var wsi=w(liquid,si);
POLY_3: ent var wmg=w(liquid,mg);
POLY_3: ent var wcu=w(liquid,cu);
POLY_3: ent tab tab1
Variable(s): t nl ns nfcc
&
POLY_3: s-c w(si)=wsi w(mg)=wmg w(cu)=wcu
POLY_3: save tcex30a y
POLY_3:
POLY_3: step
Option? /NORMAL/:  eva
Variable name(s): wsi wmg wcu
 No initial equilibrium, using default
 Global calculation of initial equilibrium ....OK

 Phase Region from    900.000     for:
     LIQUID
 Global check of adding phase at  8.97741E+02
 Calculated     5 equilibria

 Phase Region from    897.741     for:
     LIQUID
     FCC_A1
 Global test at  8.90000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  8.70000E+02 .... OK
 Global test at  8.60000E+02 .... OK
 Global check of adding phase at  8.57875E+02
 Calculated    43 equilibria

 Phase Region from    857.875     for:
     LIQUID
     FCC_A1
     MG2SI
 Global test at  8.50000E+02 .... OK
 Global test at  8.40000E+02 .... OK
 Global test at  8.30000E+02 .... OK
 Global test at  8.20000E+02 .... OK
 Global test at  8.10000E+02 .... OK
 Global test at  8.00000E+02 .... OK
 Global test at  7.90000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global check of adding phase at  7.78888E+02
 Calculated    82 equilibria

 Phase Region from    778.888     for:
     LIQUID
     ALCU_THETA
     FCC_A1
     MG2SI
 Global check of adding phase at  7.73208E+02
 Calculated     8 equilibria

 Phase Region from    773.208     for:
     LIQUID
     ALCU_THETA
     DIAMOND_A4
     FCC_A1
     MG2SI
 Calculated     2 equilibria

 Phase Region from    773.208     for:
     ALCU_THETA
     DIAMOND_A4
     FCC_A1
     MG2SI
 Global test at  7.66000E+02 .... OK
 Global test at  7.56000E+02 .... OK
 Terminating at    750.000
```

```
 Calculated    27 equilibria
 *** Buffer saved on file: tcex30a.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

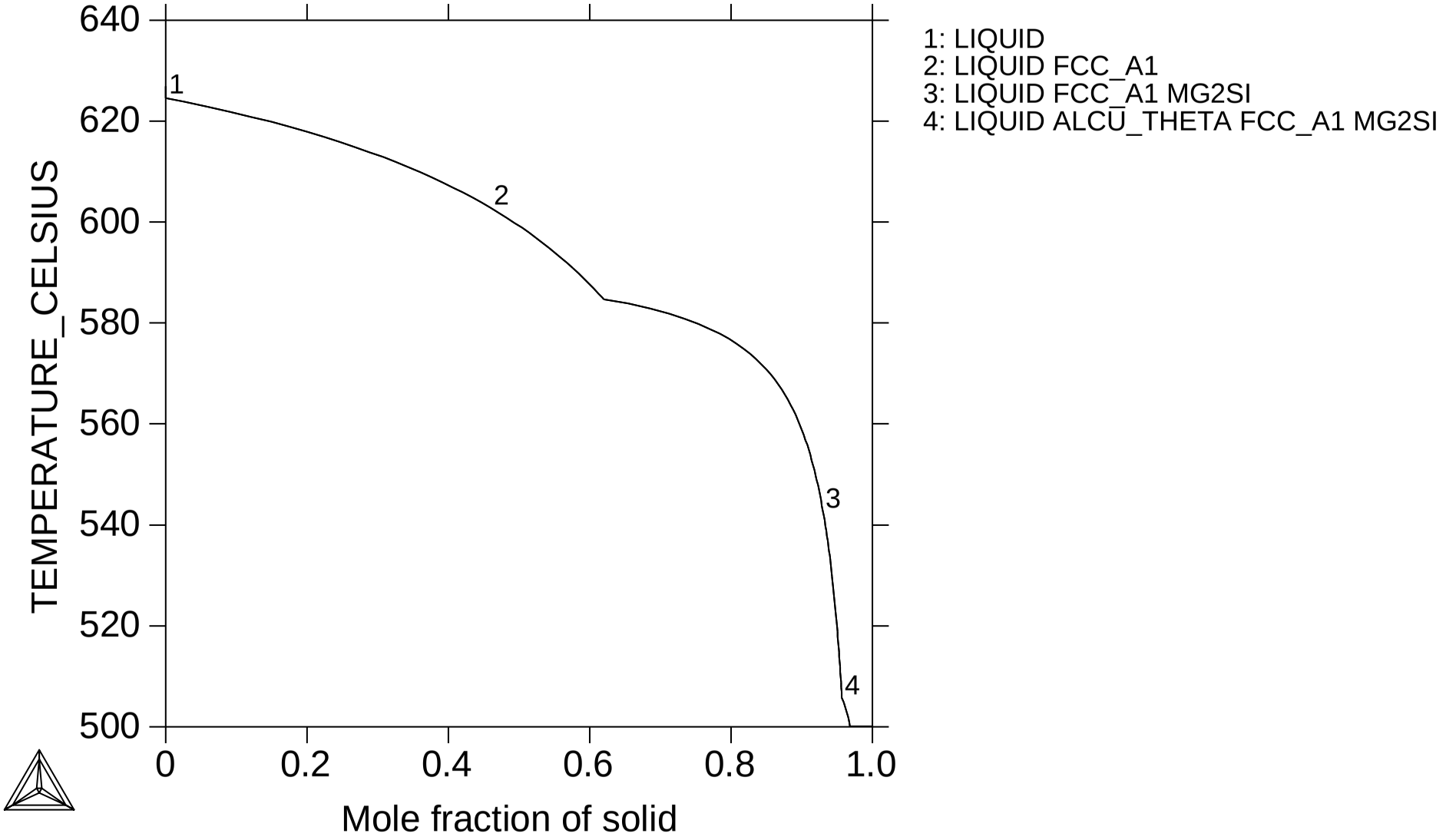
 Setting automatic diagram axis

POST: s-d-a x tab1
COLUMN NUMBER /*/:  3
POST: s-d-a y t-c
POST:
POST: s-s-s y
AUTOMATIC SCALING  (Y OR N) /N/:  n
MIN VALUE : 500 640
POST: s-lab b
POST: se-ax-te x n
AXIS TEXT : Mole fraction of solid
POST: set-title example 30Aa
POST: pl
POST:
POST:@?
POST: back
POLY_3: read,,
POLY_3: po
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

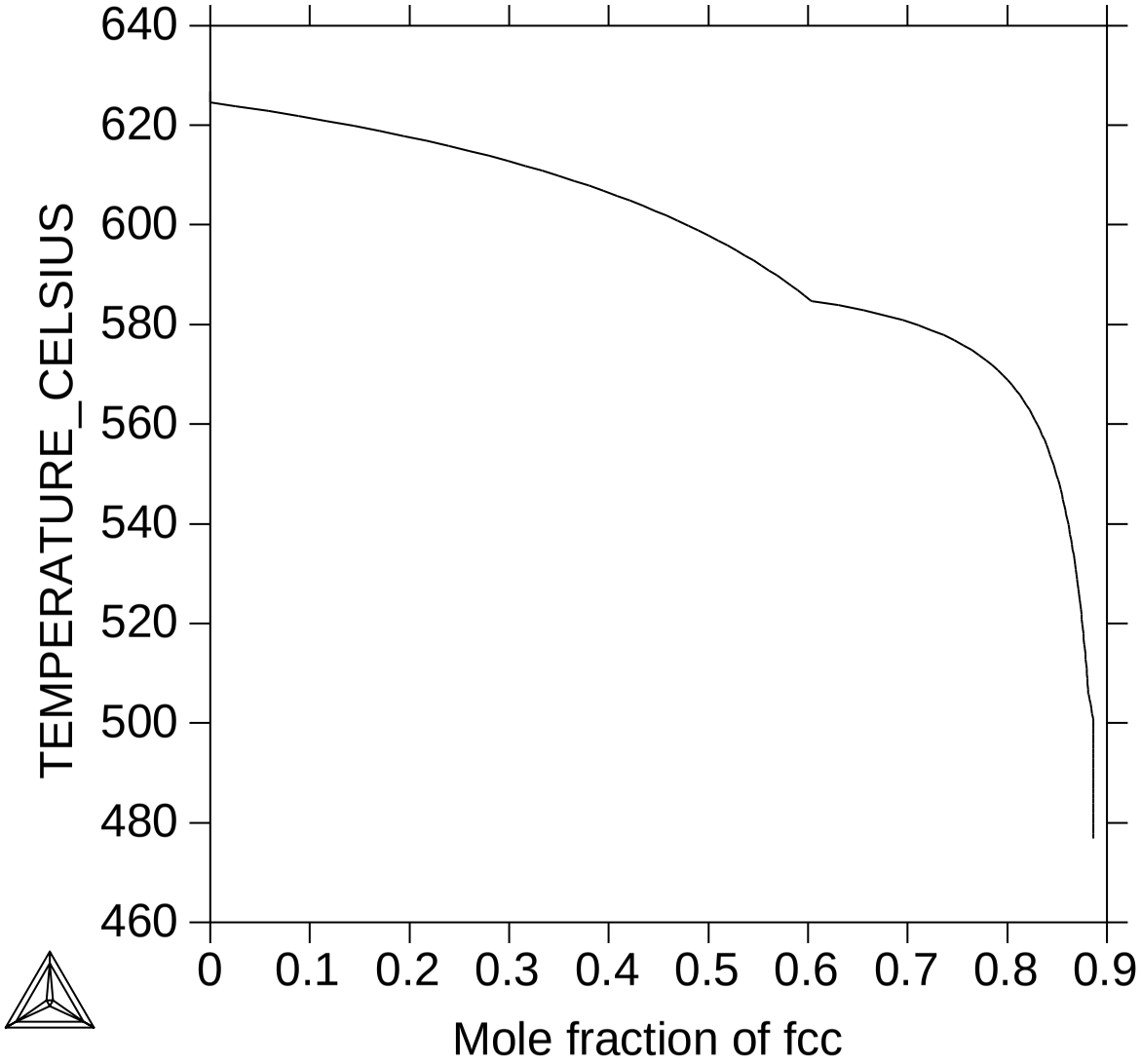
 Setting automatic diagram axis

POST: s-d-a x tab1
COLUMN NUMBER /*/:  4
POST: s-d-a y t-c
POST: se-ax-te x n
AXIS TEXT : Mole fraction of fcc
POST: set-title example 30Ab
POST: pl
POST:
POST:@?
POST: s-d-a x t-c
POST: s-d-a y w(liq,*),,
POST: set-title example 30Ac
POST: s-l d
POST: pl
POST:
POST:
POST: set-inter
POST: CPU time          10  seconds
```

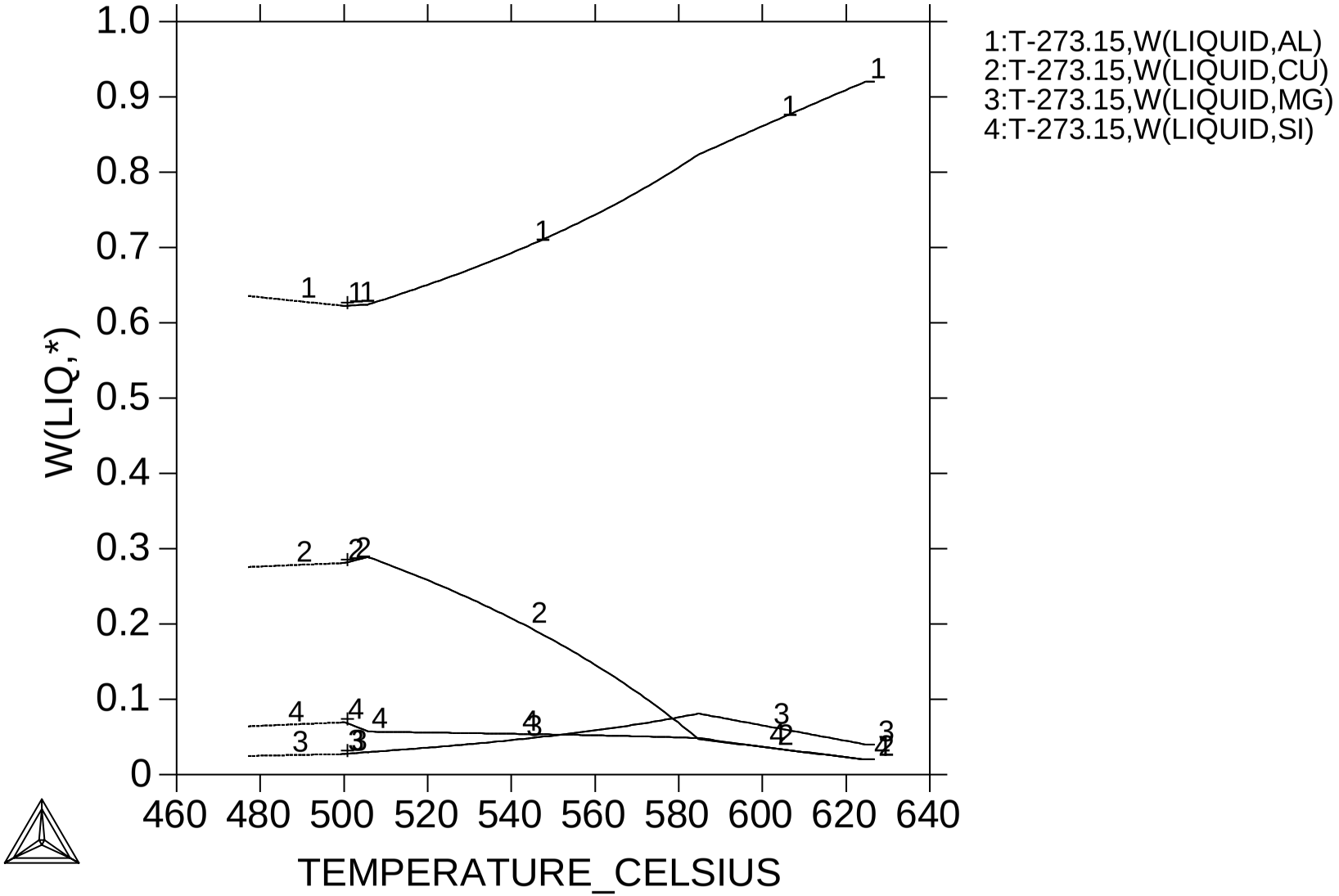
THERMO-CALC (2009.04.30:12.23) :example 30Aa
DATABASE:USER
P=1.01325E5, N=1., W(SI)=WSI, W(MG)=WMG, W(CU)=WCU;



THERMO-CALC (2009.04.30:12.23) :example 30Ab
DATABASE:USER
P=1.01325E5, N=1, W(SI)=WSI, W(MG)=WMG, W(CU)=WCU;



THERMO-CALC (2009.04.30:12.23) :example 30Ac
DATABASE:USER
P=1.01325E5, N=1, W(SI)=WSI, W(MG)=WMG, W(CU)=WCU;



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Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy

Part B. Using SCHEIL module

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example of Scheil calculation for Al-4Mg-2Si-2Cu
SYS: @@    Part B: using SCHEIL module
SYS: @@
SYS: set-log ex30,,,
SYS:
SYS: go scheil
   ... the command in full is GOTO_MODULE

         SCHEIL_GULLIVER SIMULATION MODULE VERSION 4.0

 ..........................................................
 .                                                        .
 .        1. Start new simulation                         .
 .        2. Open old file and plot diagram               .
 .        3. Open old file and make another simulation    .
 .                                                        .
 ..........................................................

Select option /1/:  1
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/:  user
FILENAME: tcex30_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
Major element or alloy: al
Composition input in mass (weight) percent? /Y/:
1st alloying element: mg 4 si 2 cu 2
Next alloying element:
Temperature (C) /2000/:  800
 VA                      /-  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 AL  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MG  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CU  DEFINED

 This database has following phases for the defined system

 LIQUID:L                AL12MG17                ALCE_AMORPHOUS
 ALCUZN_T                ALCU_DELTA              ALCU_EPSILON
 ALCU_ETA                ALCU_PRIME              ALCU_THETA
 ALCU_ZETA               ALLI                    ALMG_BETA
 ALMG_EPS                ALMG_GAMMA              ALMO
 ALM_D019                ALND_AMORPHOUS          ALTI
 BCC_A2                  BCC_B2                  BCT_A5
 CBCC_A12                CR3SI_A15               CRSI2
 CU19SI6_ETA             CU33SI7_DELTA           CU4SI_EPSILON
 CU56SI11_GAMMA          CU6Y                    CUB_A13
 CUB_A15                 CUMG2                   CUMGSI_SIGMA
 CUMGSI_TAU              CUZN_GAMMA              DIAMOND_A4
 FCC_A1                  GAMMA_D83               GAMMA_H
 HCP_A3                  HCP_ZN                  LAVES_C14
 LAVES_C15               LAVES_C36               MG24Y5
```

```
 MG2SI                  MG2Y                   MG2ZN11
 MG2ZN3                 MGY_GAMMA              MGZN
 PHI                    QPHASE                 SIV3
 SPHASE                 TAU                    VPHASE

Reject phase(s) /NONE/:  *
 LIQUID:L               AL12MG17               ALCE_AMORPHOUS
 ALCUZN_T               ALCU_DELTA             ALCU_EPSILON
 ALCU_ETA               ALCU_PRIME             ALCU_THETA
 ALCU_ZETA              ALLI                   ALMG_BETA
 ALMG_EPS               ALMG_GAMMA             ALMO
 ALM_D019               ALND_AMORPHOUS         ALTI
 BCC_A2                 BCC_B2                 BCT_A5
 CBCC_A12               CR3SI_A15              CRSI2
 CU19SI6_ETA            CU33SI7_DELTA          CU4SI_EPSILON
 CU56SI11_GAMMA         CU6Y                   CUB_A13
 CUB_A15                CUMG2                  CUMGSI_SIGMA
 CUMGSI_TAU             CUZN_GAMMA             DIAMOND_A4
 FCC_A1                 GAMMA_D83              GAMMA_H
 HCP_A3                 HCP_ZN                 LAVES_C14
 LAVES_C15              LAVES_C36              MG24Y5
 MG2SI                  MG2Y                   MG2ZN11
 MG2ZN3                 MGY_GAMMA              MGZN
 PHI                    QPHASE                 SIV3
 SPHASE                 TAU                    VPHASE
   REJECTED
Restore phase(s)::  liq fcc alcu_th mg2si dia al12mg17
 LIQUID:L               FCC_A1                 ALCU_THETA
 MG2SI                  DIAMOND_A4             AL12MG17
   RESTORED
Restore phase(s): /NONE/:

 .....................................................

    The following phases are retained in this system:

 LIQUID:L               AL12MG17               ALCU_THETA
 DIAMOND_A4             FCC_A1                 MG2SI

 .....................................................

OK? /Y/:  Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 Reference REF1       missing
 Reference REF1       missing
 Reference REF1       missing
 Reference REF1       missing
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
 -OK-
Should any phase have a miscibility gap check? /N/:  N
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
     Calculated liquidus temperature is  625.00(C)
     Please enter simulation conditions !

Temperature step (C) /1/:  1
Default stop point? /Y/:  Y
Fast diffusing components: /NONE/:
Buffer-saving file name /scheil/:
   ... the command in full is ADD_INITIAL_EQUILIBRIUM

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.
```

```
  ... the command in full is ADVANCED_OPTIONS
  ... the command in full is STEP_WITH_OPTIONS

Phase Region from    898.150     for:
    LIQUID
Calculated     4 equilibria

Phase Region from    897.741     for:
    LIQUID
    FCC_A1
Calculated    43 equilibria

Phase Region from    857.535     for:
    LIQUID
    FCC_A1
    MG2SI
Calculated    34 equilibria

Phase Region from    826.196     for:
    FCC_A1
    MG2SI
*** Buffer saved on file: scheil.POLY3

 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

  ... the command in full is ENTER_SYMBOL
  ... the command in full is MAKE_EXPERIMENTAL_DATAFI
An EXP file scheil_EQ.EXP
has been created to store the equilibrium            solidification results.
  ... the command in full is READ_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

  ... the command in full is ADD_INITIAL_EQUILIBRIUM

      :
      :
      :

Phase Region from    857.875     for:
    LIQUID
    FCC_A1
    MG2SI
Calculated    82 equilibria

Phase Region from    778.888     for:
    LIQUID
    ALCU_THETA
    FCC_A1
    MG2SI

Phase Region from    773.208     for:
    LIQUID
    ALCU_THETA
    DIAMOND_A4
    FCC_A1
    MG2SI
Calculated     8 equilibria

Phase Region from    773.208     for:
    ALCU_THETA
    DIAMOND_A4
    FCC_A1
    MG2SI
Calculated     3 equilibria
```

```
 *** Buffer saved on file: scheil.POLY3
   ... the command in full is REINITIATE_PLOT_SETTINGS

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is SET_AUTOMATIC_DIAGRAM_A

 Setting automatic diagram axis

   ... the command in full is APPEND_EXPERIMENTAL_DATA
Hard copy of the diagram? /N/:  n
Save coordinates of curve on text file? /N/:  n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
   ... the command in full is SET_LABEL_CURVE_OPTION
Any more diagrams? /Y/:

  ..........................................................

        The following axis variables are available

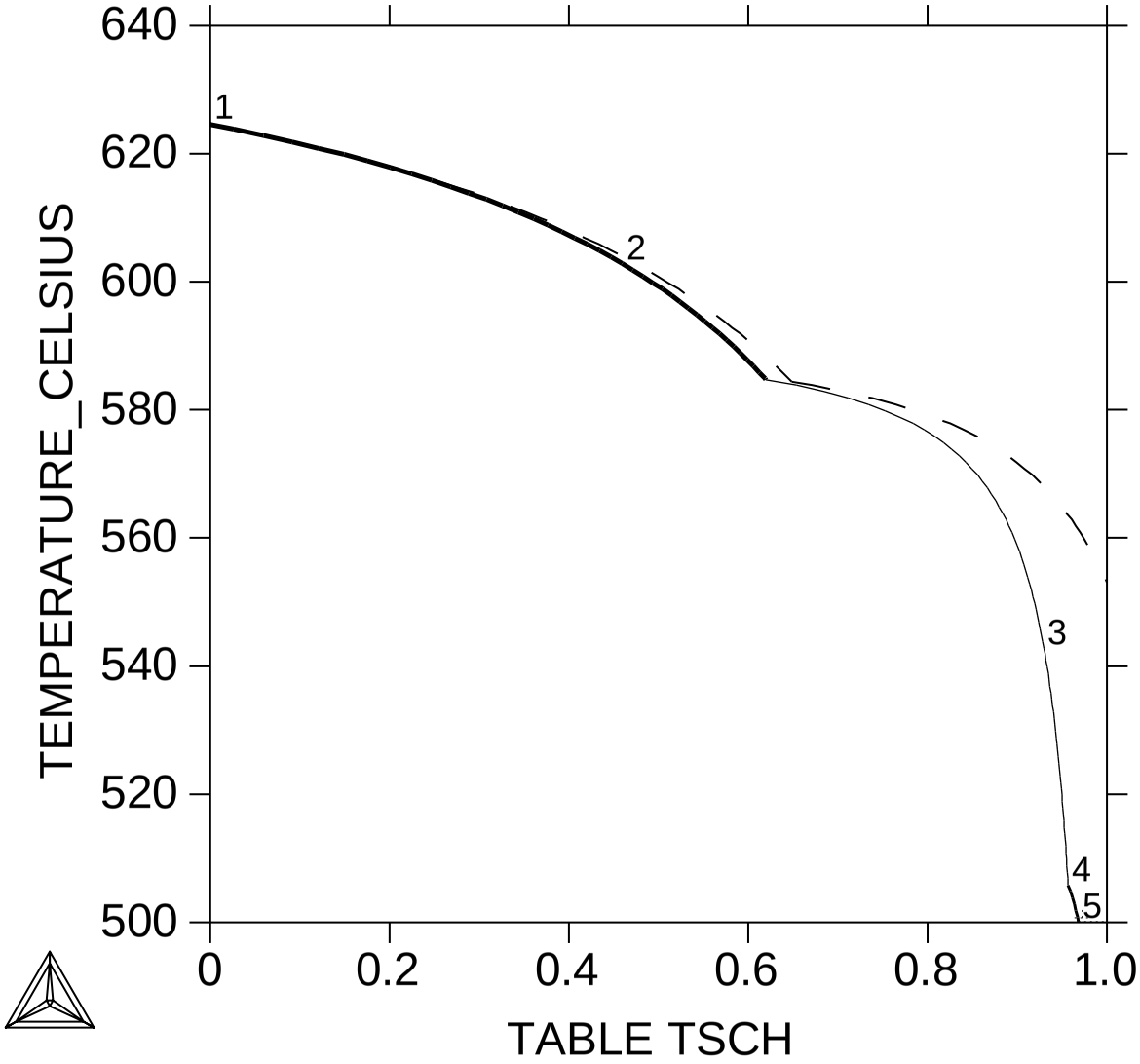
             T --- Temperature in Celsius
         NL/BL --- Mole/mass fraction of liquid
         NS/BS --- Mole/mass fraction of all solid phases
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
      W(ph,el) --- Weight fraction of an element in a phase
      X(ph,el) --- Mole fraction of an element in a phase
      Y(ph,el) --- Site fraction of an element in a phase
     NN(ph,el) --- Distribution of an element in a phases
         NH/BH --- Heat release and Latent heat per mole/gram
        CP/BCP --- Apparent heat capacity per mole/gram

  "el" and "ph" are name of element and phase, respectively
     "*" can be used as a wild character for "el" and "ph"

  ..........................................................

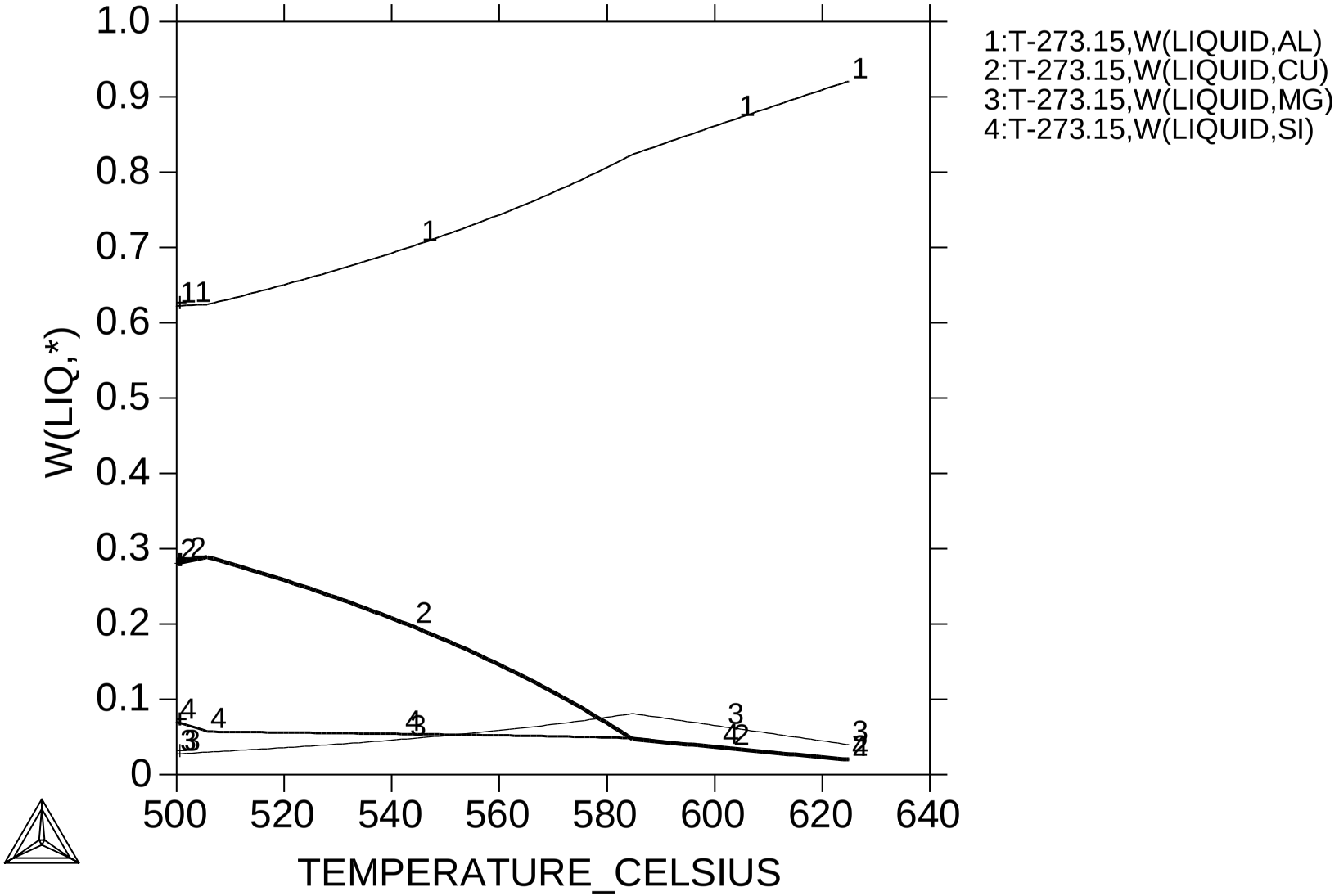
X-axis Variable: t
Y-axis Variable: w(liq,*)
Zoom in? /N/:  y
Change scaling of X-axis? /Y/:  n
Change scaling of Y-axis? /Y/:  y
Minimum /0/:  0
Maximum /1/:  .3
Zoom in? /N/:  n
Hard copy of the diagram? /N/:  n
Save coordinates of curve on text file? /N/:  n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
   ... the command in full is SET_LABEL_CURVE_OPTION
Any more diagrams? /Y/:  n
   ... the command in full is ADVANCED_OPTIONS
SYS:
SYS: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
SYS:SYS: CPU time           1  seconds
```

THERMO-CALC (2009.04.22:17.33) :example 30Ba
DATABASE:USER
W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=1E5, N=1;

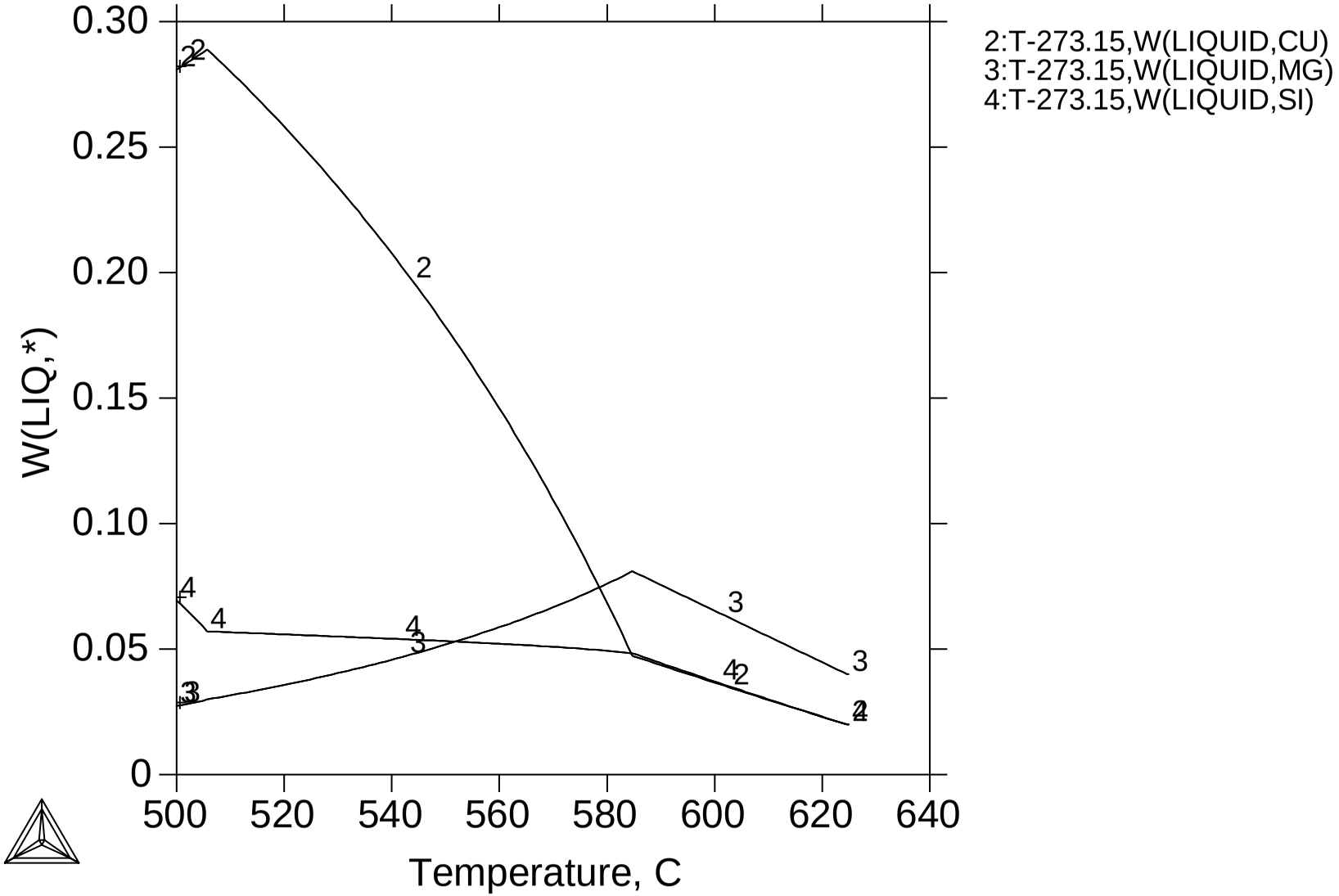


1: LIQUID
2: LIQUID FCC_A1
3: LIQUID FCC_A1 MG2SI
4: LIQUID ALCU_THETA FCC_A1 MG2SI
5: LIQUID ALCU_THETA DIAMOND_A4 FCC_A1 M

THERMO-CALC (2009.04.22:17.35) :example 30Bb
DATABASE:USER
W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=1E5, N=1;



THERMO-CALC (2009.04.22:17.59) :example 30Bc
DATABASE:USER
W(MG)=WMG, W(SI)=WSI, W(CU)=WCU, P=1E5, N=1;



31

CVM calculation

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculations of CVM and comparisons with sublattices
SYS: @@ of a fictitious A B system.
SYS: @@ Also shows how to overlay diagrams from two calculations
SYS: @@
SYS:
SYS: set-log ex31,,,
SYS:
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
 First version released 1-Jan-78, last update 20-Nov-2007

GES:
GES: @@ Enter the elements and their reference states
GES: e-e A B
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
GES: a-e-d A
   ... the command in full is AMEND_ELEMENT_DATA
NEW STABLE ELEMENT REFERENCE /UNKNOWN/:  FCC
NEW ATOMIC MASS /0/:  10
NEW H(298.15)-H(0) /0/:  0
NEW S(298.15) /0/:  0
Default element reference state symbol index /1/:  1
GES: a-e-d B
   ... the command in full is AMEND_ELEMENT_DATA
NEW STABLE ELEMENT REFERENCE /BETA_RHOMBO_B/:  FCC
NEW ATOMIC MASS /10.811/:  10
NEW H(298.15)-H(0) /1222/:  0
NEW S(298.15) /5.9/:  0
Default element reference state symbol index /1/:  1
GES:
GES: @@ ====================================================
GES: @@ These species represent the clusters. 4 clusters A3B are needed
GES: @@ as the B atom can be on 4 different sublattices etc.
GES: e-sp S0 A
   ... the command in full is ENTER_SPECIES
GES: e-sp S11 A.75B.25
   ... the command in full is ENTER_SPECIES
GES: e-sp S12 A.75B.25
   ... the command in full is ENTER_SPECIES
GES: e-sp S13 A.75B.25
   ... the command in full is ENTER_SPECIES
GES: e-sp S14 A.75B.25
   ... the command in full is ENTER_SPECIES
GES: e-sp S21 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S22 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S23 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S24 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S25 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S26 A.5B.5
   ... the command in full is ENTER_SPECIES
GES: e-sp S31 A.25B.75
   ... the command in full is ENTER_SPECIES
```

GES: **e-sp S32 A.25B.75**
... the command in full is ENTER_SPECIES
GES: **e-sp S33 A.25B.75**
... the command in full is ENTER_SPECIES
GES: **e-sp S34 A.25B.75**
... the command in full is ENTER_SPECIES
GES: **e-sp S4 B**
... the command in full is ENTER_SPECIES
GES:
GES: *@@ ==========*
GES: *@@ **This function describes the bond energy A-B at equiatomic composition***
GES: **e-sy fun UIJ**
... the command in full is ENTER_SYMBOL
LOW TEMPERATURE LIMIT /298.15/: **298.15**
FUNCTION: **-100*R;**
HIGH TEMPERATURE LIMIT /6000/: **6000**
ANY MORE RANGES /N/: **N**
GES:
GES: *@@ **These functions describe the end-member energies at A3B, A2B2 and AB3***
GES: *@@ **respectivly. In the simplest case, like here, they are just the***
GES: *@@ **bond energy multiplied with 3, 4 and 3 respectively.***
GES: **e-sy fun GA3B1,,3*UIJ;,,,**
... the command in full is ENTER_SYMBOL
GES: **e-sy fun GA2B2,,4*UIJ;,,,**
... the command in full is ENTER_SYMBOL
GES: **e-sy fun GA1B3,,3*UIJ;,,,**
... the command in full is ENTER_SYMBOL
GES:
GES: *@@ ==========*
GES: *@@ **This is the fcc phase with CVM for both lro and sro***
GES: **e-ph CVM_TET**
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: **1**
NAME OF CONSTITUENT: **S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34**
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: **NO**
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: **NO**
GES: **E-PAR G(C,S11),,GA3B1;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: **E-PAR G(C,S12),,GA3B1;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: **E-PAR G(C,S13),,GA3B1;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: **E-PAR G(C,S14),,GA3B1;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: **E-PAR G(C,S21),,GA2B2;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: **E-PAR G(C,S22),,GA2B2;,,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: **E-PAR G(C,S23),,GA2B2;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: **E-PAR G(C,S24),,GA2B2;,,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: **E-PAR G(C,S25),,GA2B2;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: **E-PAR G(C,S26),,GA2B2;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: **E-PAR G(C,S31),,GA1B3;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: **E-PAR G(C,S32),,GA1B3;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)

GES: **E-PAR G(C,S33),,GA1B3;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: **E-PAR G(C,S34),,GA1B3;,,,**
... the command in full is ENTER_PARAMETER
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: **l-d,,,,**
... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH DATE 2009- 4-15
FROM DATABASE: User data 2009. 4.15

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE ELEMENT REFERENCE	MASS	H298-H0	S298
1 A	FCC	1.0000E+01	0.0000E+00	0.0000E+00
2 B	FCC	1.0000E+01	0.0000E+00	0.0000E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 S0	A
4 S11	A0.75B0.25
5 S12	A0.75B0.25
6 S13	A0.75B0.25
7 S14	A0.75B0.25
8 S21	A0.5B0.5
9 S22	A0.5B0.5
10 S23	A0.5B0.5
11 S24	A0.5B0.5
12 S25	A0.5B0.5
13 S26	A0.5B0.5
14 S31	A0.25B0.75
15 S32	A0.25B0.75
16 S33	A0.25B0.75
17 S34	A0.25B0.75
18 S4	B

CVM_TET
CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
S4

G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
103 UIJ	20000000	-100*R
104 GA3B1	20000000	+3*UIJ
105 GA2B2	20000000	+4*UIJ
106 GA1B3	20000000	+3*UIJ

GES:
GES: **@?<Hit_return_to_continue>**
GES: ***@@ ==***
GES: ***@@ This is an fcc phase with no sro but lro***
GES: ***@@ described with the sublattice model***
GES: **E-PH LRO**

```
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/:  4
NUMBER OF SITES IN SUBLATTICE  1 /1/:  .25
NUMBER OF SITES IN SUBLATTICE  2 /1/:  .25
NUMBER OF SITES IN SUBLATTICE  3 /1/:  .25
NUMBER OF SITES IN SUBLATTICE  4 /1/:  .25
 CONSTITUENTS IN SUBLATTICE           1
NAME OF CONSTITUENT: A B;
 CONSTITUENTS IN SUBLATTICE           2
NAME OF CONSTITUENT: A B;
 CONSTITUENTS IN SUBLATTICE           3
NAME OF CONSTITUENT: A B;
 CONSTITUENTS IN SUBLATTICE           4
NAME OF CONSTITUENT: A B;
WILL YOU ADD CONSTITUENTS LATER /NO/:  NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/:  NO
GES:
GES: E-PAR G(L,A:A:A:B),,GA3B1;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(L,A:A:B:A),,GA3B1;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(L,A:B:A:A),,GA3B1;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:B:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(L,B:A:A:A),,GA3B1;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(L,A:B:B:B),,GA1B3;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:B:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(L,B:A:B:B),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(L,B:B:A:B),,GA1B3;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:B:A:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(L,B:B:B:A),,GA1B3;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:B:B:A;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(L,A:A:B:B),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,A:B:A:B),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,B:A:A:B),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:A:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,A:B:B:A),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,A:B:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,B:A:B:A),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(L,B:B:A:A),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: l-p-d lro
   ... the command in full is LIST_PHASE_DATA

 LRO
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: A,B : A,B : A,B : A,B

      G(LRO,A:A:A:A;0)-G(FCC,A;0) = 0.0
      G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(LRO,A:B:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
```

```
      G(LRO,A:B:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(LRO,B:B:B:A;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(LRO,A:A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(LRO,B:A:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(LRO,A:B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(LRO,B:B:A:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(LRO,A:B:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(LRO,B:B:B:B;0)-G(FCC,B;0) = 0.0
GES:
GES: @@ ============================================================
GES: @@ This is the fcc phase with no sro and no lro.  The regular
GES: @@ parameters is simply 12 times the bond energy as the ;1 and ;2
GES: @@ parameters cancel when GA1B3=GA3B1=0.75*GA2B2
GES: e-ph fcc_a1
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/:  1
NAME OF CONSTITUENT: A B
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/:  NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/:  NO
GES:
GES: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;0)
GES: e-par l(fcc,a,b;1),,2*GA3B1-2*GA1B3;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;1)
GES: e-par l(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3;,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;2)
GES: l-p-d fcc
   ... the command in full is LIST_PHASE_DATA

 FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
      G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
      L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
      L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3
      L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3
GES:
GES: @@ Finally we add together the LRO phase with the disordered FCC
GES: @@ Note that the parameters in LRO will give zero contribution
GES: @@ when the phase is disordered
GES: amend-phase LRO dis FCC
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: @@
GES: @@ This is the secret way to set CVM entropy calculation
GES: am-ph cvm stat 02204030
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: l-p-d cvm
   ... the command in full is LIST_PHASE_DATA

 CVM_TET
 $ CVM-SRO ENTROPY CONTRIBUTION
    CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
    S4

      G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
      G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
```

```
      G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0
GES:
GES: @?<Hit_return_to_continue>
GES: @@ We need 3 CVM phases for the L10, L12 and disordered states
GES: am-ph cvm
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER /2/: 3
 GIVE FOR COMPOSITION SET           2
Major constituent(s) for sublattice 1: /$/: s11
 GIVE FOR COMPOSITION SET           3
Major constituent(s) for sublattice 1: /$/: none
GES:
GES: am-ph cvm maj
   ... the command in full is AMEND_PHASE_DESCRIPTION
Composition set /1/: 1
Major constituent(s) for sublattice 1: /S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S/: S25
GES:
GES: @@ Also for the sublattice phase we need 3 composition sets
GES: am-ph lro
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER /2/: 3
 GIVE FOR COMPOSITION SET           2
Major constituent(s) for sublattice 1: /A B/: *
Major constituent(s) for sublattice 2: /A B/: *
Major constituent(s) for sublattice 3: /A B/: *
Major constituent(s) for sublattice 4: /A B/: *
 GIVE FOR COMPOSITION SET           3
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: B
Major constituent(s) for sublattice 4: /A B/: B
GES: am-ph lro
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: maj
Composition set /1/: 1
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: A
Major constituent(s) for sublattice 4: /A B/: B
GES:
GES: l-d,,,,
   ... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH          DATE 2009- 4-15
 FROM DATABASE: User data 2009. 4.15

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  1 A    FCC                      1.0000E+01  0.0000E+00  0.0000E+00
  2 B    FCC                      1.0000E+01  0.0000E+00  0.0000E+00

 SPECIES                                   STOICHIOMETRY
   1 A                                     A
   2 B                                     B
   3 S0                                    A
   4 S11                                   A0.75B0.25
   5 S12                                   A0.75B0.25
   6 S13                                   A0.75B0.25
   7 S14                                   A0.75B0.25
   8 S21                                   A0.5B0.5
   9 S22                                   A0.5B0.5
  10 S23                                   A0.5B0.5
  11 S24                                   A0.5B0.5
  12 S25                                   A0.5B0.5
```

```
 13 S26                                    A0.5B0.5
 14 S31                                    A0.25B0.75
 15 S32                                    A0.25B0.75
 16 S33                                    A0.25B0.75
 17 S34                                    A0.25B0.75
 18 S4                                     B

 CVM_TET
 $ CVM-SRO ENTROPY CONTRIBUTION
    CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
    S4

      G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
      G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
      G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
      G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
      G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0

 FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF LRO
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
      G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
      L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
      L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3
      L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3

 LRO
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: A,B : A,B : A,B : A,B

      G(LRO,A:A:A:A;0) = 0.0
      G(LRO,B:A:A:A;0) = +GA3B1
      G(LRO,A:B:A:A;0) = +GA3B1
      G(LRO,B:B:A:A;0) = +GA2B2
      G(LRO,A:A:B:A;0) = +GA3B1
      G(LRO,B:A:B:A;0) = +GA2B2
      G(LRO,A:B:B:A;0) = +GA2B2
      G(LRO,B:B:B:A;0) = +GA1B3
      G(LRO,A:A:A:B;0) = +GA3B1
      G(LRO,B:A:A:B;0) = +GA2B2
      G(LRO,A:B:A:B;0) = +GA2B2
      G(LRO,B:B:A:B;0) = +GA1B3
      G(LRO,A:A:B:B;0) = +GA2B2
      G(LRO,B:A:B:B;0) = +GA1B3
      G(LRO,A:B:B:B;0) = +GA1B3
      G(LRO,B:B:B:B;0) = 0.0

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 103 UIJ       20000000 -100*R
 104 GA3B1     20000000 +3*UIJ
 105 GA2B2     20000000 +4*UIJ
 106 GA1B3     20000000 +3*UIJ

GES: @?<Hit_return_to_continue>
GES: @@ ========================================
GES: @@ Now we can start calculating
```

```
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3:
POLY_3: @@ turn global minimization off
POLY_3: set-min-op
   ... the command in full is SET_MINIMIZATION_OPTIONS
 This command is DEPRECATED and to be removed in the future!
 Settings for global minimization:
 Use global minimization /Y/:  n
 Settings for general calculations:
 Force positive definite Phase Hessian /Y/:  n
 Control minimization step size /Y/:
POLY_3:
POLY_3: L-C
   ... the command in full is LIST_CONDITIONS
 DEGREES OF FREEDOM 4
POLY_3: S-C T=60 P=1E5 N=1 X(B)=.4
   ... the command in full is SET_CONDITION
POLY_3: @@
POLY_3: @@ First calculate just with the full CVM phases
POLY_3: ch-st ph *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: ch-st ph cvm cvm#2 cvm#3=ent 1
   ... the command in full is CHANGE_STATUS
POLY_3: @@
POLY_3: @@ L10 ordering, setting start composition essential ....
POLY_3: @@ The initial fraction of each species is bascially calculated as the
POLY_3: @@ product of the site fraction on each sublattice.
POLY_3: s-s-c cvm
   ... the command in full is SET_START_CONSTITUTION
Y(CVM_TET#1,S0) /1/:  .002
Y(CVM_TET#1,S11) /1/:  1.16e-3
Y(CVM_TET#1,S12) /1/:  1.76e-1
Y(CVM_TET#1,S13) /1/:  1.16e-3
Y(CVM_TET#1,S14) /1/:  1.76e-1
Y(CVM_TET#1,S21) /1/:  7.56e-3
Y(CVM_TET#1,S22) /1/:  5e-5
Y(CVM_TET#1,S23) /1/:  7.56e-3
Y(CVM_TET#1,S24) /1/:  7.56e-3
Y(CVM_TET#1,S25) /1/:  6.08e-1
Y(CVM_TET#1,S26) /1/:  7.56e-3
Y(CVM_TET#1,S31) /1/:  1.76e-3
Y(CVM_TET#1,S32) /1/:  2e-5
Y(CVM_TET#1,S33) /1/:  1.76e-3
Y(CVM_TET#1,S34) /1/:  2e-5
Y(CVM_TET#1,S4) /1/:  4e-7
POLY_3:
POLY_3: @@ L12 ordering
POLY_3: s-s-c cvm#2
   ... the command in full is SET_START_CONSTITUTION
Y(CVM_TET#2,S0) /1/:  .002
Y(CVM_TET#2,S11) /1/:  .46
Y(CVM_TET#2,S12) /1/:  .0078
Y(CVM_TET#2,S13) /1/:  .0078
Y(CVM_TET#2,S14) /1/:  .0078
Y(CVM_TET#2,S21) /1/:  .168
Y(CVM_TET#2,S22) /1/:  .168
Y(CVM_TET#2,S23) /1/:  .168
Y(CVM_TET#2,S24) /1/:  .0012
Y(CVM_TET#2,S25) /1/:  .0012
Y(CVM_TET#2,S26) /1/:  .0012
Y(CVM_TET#2,S31) /1/:  5e-6
Y(CVM_TET#2,S32) /1/:  .002
Y(CVM_TET#2,S33) /1/:  .002
Y(CVM_TET#2,S34) /1/:  .002
Y(CVM_TET#2,S4) /1/:  1e-6
POLY_3:
POLY_3: s-s-c cvm#3 *
   ... the command in full is SET_START_CONSTITUTION
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
```

```
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    19 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  xnp
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=60, P=1E5, N=1, X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     60.00 K (  -213.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.10213E+03,  Enthalpy -2.96850E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 2.0465E-02 -1.9401E+03 SER
 B                       4.0000E-01  4.0000E-01 6.0538E-05 -4.8452E+03 SER

 CVM_TET#1                   Status ENTERED     Driving force  0.0000E+00
 Moles 5.6950E-01, Mass 5.6950E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  5.89207E-01  B  4.10793E-01
 Constitution:
 S25  5.78440E-01  S23  1.28068E-02  S33  4.13398E-03  S22  2.56479E-04
 S14  1.76120E-01  S21  1.28068E-02  S0   3.76373E-03  S32  1.15932E-04
 S12  1.76120E-01  S24  1.28068E-02  S13  2.78465E-03  S34  1.15932E-04
 S26  1.28068E-02  S31  4.13398E-03  S11  2.78465E-03  S4   3.67798E-06

 CVM_TET#2                   Status ENTERED     Driving force  0.0000E+00
 Moles 4.3050E-01, Mass 4.3050E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.14278E-01  B  3.85722E-01
 Constitution:
 S11  4.21306E-01  S12  1.38900E-02  S34  4.69234E-03  S25  3.19866E-03
 S21  1.69717E-01  S13  1.38900E-02  S32  4.69234E-03  S26  3.19866E-03
 S22  1.69717E-01  S14  1.38900E-02  S0   4.13973E-03  S31  5.05554E-05
 S23  1.69717E-01  S33  4.69234E-03  S24  3.19866E-03  S4   8.90403E-06

 CVM_TET#3                   Status ENTERED     Driving force -1.0709E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.09450E-01  B  3.90550E-01
 Constitution:
 S14  1.09230E-01  S26  8.47466E-02  S24  8.47466E-02  S32  8.87560E-03
 S13  1.09230E-01  S23  8.47466E-02  S25  8.47466E-02  S33  8.87560E-03
 S11  1.09230E-01  S22  8.47466E-02  S0   1.86436E-02  S34  8.87560E-03
 S12  1.09230E-01  S21  8.47466E-02  S31  8.87560E-03  S4   4.53364E-04
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-c t=40
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    18 ITS,  CPU TIME USED   0 SECONDS
POLY_3: s-s-c cvm#3 *
   ... the command in full is SET_START_CONSTITUTION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    18 ITS,  CPU TIME USED   0 SECONDS
POLY_3: L-E
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VXNP/:
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=40, P=1E5, N=1, X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     40.00 K (  -233.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.06232E+03,  Enthalpy -2.98938E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 4.1519E-03 -1.8239E+03 SER
```

```
 B                      4.0000E-01  4.0000E-01 3.7621E-07 -4.9199E+03 SER

 CVM_TET#1                   Status ENTERED     Driving force  0.0000E+00
 Moles 6.6953E-01, Mass 6.6953E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  5.88358E-01  B  4.11642E-01
 Constitution:
 S25  6.26368E-01  S26  4.57470E-03  S33  6.44301E-04  S22  1.02379E-05
 S12  1.76201E-01  S24  4.57470E-03  S31  6.44301E-04  S32  4.02672E-06
 S14  1.76201E-01  S23  4.57470E-03  S11  4.60814E-04  S34  4.02672E-06
 S21  4.57470E-03  S0   7.03194E-04  S13  4.60814E-04  S4   2.24689E-08

 CVM_TET#2                   Status ENTERED     Driving force  0.0000E+00
 Moles 3.3047E-01, Mass 3.3047E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.23586E-01  B  3.76414E-01
 Constitution:
 S11  4.81572E-01  S14  4.56422E-03  S33  7.57611E-04  S25  4.03145E-04
 S23  1.66859E-01  S13  4.56422E-03  S34  7.57611E-04  S24  4.03145E-04
 S22  1.66859E-01  S12  4.56422E-03  S0   6.77145E-04  S31  4.66624E-07
 S21  1.66859E-01  S32  7.57611E-04  S26  4.03145E-04  S4   4.50770E-08

 CVM_TET#3                   Status ENTERED     Driving force -3.4466E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.15550E-01  B  3.84450E-01
 Constitution:
 S14  1.12327E-01  S26  8.23389E-02  S21  8.23389E-02  S33  8.17828E-03
 S13  1.12327E-01  S23  8.23389E-02  S22  8.23389E-02  S34  8.17828E-03
 S12  1.12327E-01  S24  8.23389E-02  S0   2.33728E-02  S31  8.17828E-03
 S11  1.12327E-01  S25  8.23389E-02  S32  8.17828E-03  S4   5.71422E-04
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-a-v 1 x(b) 0 .5,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 0 100,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex31a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map -
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.116E-01  4.000E+01
     CVM_TET#1
  ** CVM_TET#2
 *** Buffer saved on file: tcex31a.POLY3
 Terminating at diagram limit
 CALCULATED    27 EQUILIBRIA

 Phase region boundary   2 at:   4.116E-01  4.000E+01
     CVM_TET#1
  ** CVM_TET#2
 CALCULATED    26 EQUILIBRIA

 Phase region boundary   2 at:   4.240E-01  8.061E+01
     CVM_TET#1
  ** CVM_TET#2
     CVM_TET#3

 Phase region boundary   2 at:   4.147E-01  8.061E+01
  ** CVM_TET#2
     CVM_TET#3
 *** SORRY CANNOT CONTINUE ***    4

 CALCULATED    95 EQUILIBRIA

 Phase region boundary   2 at:   4.240E-01  8.061E+01
     CVM_TET#1
  ** CVM_TET#3
 Terminating at diagram limit
 CALCULATED    24 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE: tcex31a.POLY3
```

```
 CPU time for mapping           4  seconds
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x m-f b
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 31a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Make an experimental data file to overlay the next calculation
POST: make tcex31 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY_3: @@
POLY_3: @@ It is interesting to compare with a CEF without any sro contribution.
POLY_3: @@ This is the classical FCC ordering diagram first calculated
POLY_3: @@ manually by W Shockley, J chem Phys, 6, (1938) p 130
POLY_3: read tcex31a
   ... the command in full is READ_WORKSPACES
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p lro lro#2 lro#3=ent 0
   ... the command in full is CHANGE_STATUS
POLY_3: s-c t=70 x(b)=.4
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    32 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=70, P=1E5, N=1., X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     70.00 K (  -203.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.08055E+03,  Enthalpy -2.95310E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 4.7333E-02 -1.7755E+03 SER
 B                       4.0000E-01  4.0000E-01 1.7400E-04 -5.0382E+03 SER

 LRO#1                        Status ENTERED     Driving force  0.0000E+00
 Moles 2.6762E-01, Mass 2.6762E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.74559E-01  B  3.25441E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99692E-01  A  3.08116E-04
```

```
 LRO#2                       Status ENTERED     Driving force -4.6485E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.45965E-01  B  3.54035E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01

 LRO#3                       Status ENTERED     Driving force  0.0000E+00
 Moles 7.3238E-01, Mass 7.3238E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  5.72756E-01  B  4.27244E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.99661E-01  B  3.38612E-04
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.99661E-01  B  3.38612E-04
 Sublattice  3,  Number of sites  2.5000E-01
 B  8.54150E-01  A  1.45850E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  8.54150E-01  A  1.45850E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-s-c lro#3
   ... the command in full is SET_START_CONSTITUTION
Y(LRO#3,A) /.9996613878/:
Y(LRO#3,B) /3.386121641E-04/:
Y(LRO#3,A#2) /.9996613878/:
Y(LRO#3,B#2) /3.386121641E-04/:
Y(LRO#3,A#3) /.1458499446/:  0.0001
Y(LRO#3,B#3) /.8541500554/:  0.9999
Y(LRO#3,A#4) /.1458499446/:  .6
Y(LRO#3,B#4) /.8541500554/:  .4
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    23 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=70, P=1E5, N=1., X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     70.00 K (  -203.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.09267E+03,  Enthalpy -2.98506E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 4.1721E-02 -1.8489E+03 SER
 B                       4.0000E-01  4.0000E-01 1.9961E-04 -4.9583E+03 SER

 LRO#1                       Status ENTERED     Driving force -3.9691E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.68667E-01  B  3.31333E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99690E-01  A  3.09928E-04

 LRO#2                       Status ENTERED     Driving force -4.9687E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.39146E-01  B  3.60854E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
```

```
 A  6.39146E-01  B  3.60854E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01

 LRO#3                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  6.00000E-01  B  4.00000E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.98449E-01  B  1.55066E-03
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.98449E-01  B  1.55066E-03
 Sublattice  3,  Number of sites  2.5000E-01
 B  9.92271E-01  A  7.72920E-03
 Sublattice  4,  Number of sites  2.5000E-01
 B  6.04628E-01  A  3.95372E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-c x(b)=.33
   ... the command in full is SET_CONDITION
POLY_3: s-s-c lro *
   ... the command in full is SET_START_CONSTITUTION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    23 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=70, P=1E5, N=1., X(B)=0.33
 DEGREES OF FREEDOM 0

 Temperature     70.00 K (  -203.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -2.85605E+03,  Enthalpy -2.74060E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.7000E-01  6.7000E-01 5.7336E-02 -1.6639E+03 SER
 B                       3.3000E-01  3.3000E-01 1.1554E-04 -5.2765E+03 SER

 LRO#1                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.8876E-02, Mass 7.8876E-01, Volume fraction 0.0000E+00  Mole fractions:
 A  6.87496E-01  B  3.12504E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.16558E-01  B  8.34422E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.16558E-01  B  8.34422E-02
 Sublattice  3,  Number of sites  2.5000E-01
 A  9.16558E-01  B  8.34422E-02
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99689E-01  A  3.11152E-04

 LRO#2                      Status ENTERED     Driving force -4.8130E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.61498E-01  B  3.38502E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01

 LRO#3                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.2112E-01, Mass 9.2112E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.68502E-01  B  3.31498E-01
 Constitution:
```

```
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.82295E-01  B  1.77045E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.82295E-01  B  1.77045E-02
 Sublattice  3,  Number of sites  2.5000E-01
 B  9.99255E-01  A  7.44800E-04
 Sublattice  4,  Number of sites  2.5000E-01
 A  7.08671E-01  B  2.91329E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-a-v 2 t 0 250 5
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: save tcex31c y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: add -1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  -1  T=70, P=100000, N=1., X(B)=0.33
POLY_3:
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: map -
 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   3.315E-01  7.000E+01
  ** LRO#1
     LRO#3
 *** SORRY CANNOT CONTINUE ***    4

 CALCULATED    41 EQUILIBRIA

 Phase region boundary   2 at:   3.315E-01  7.000E+01
  ** LRO#1
     LRO#3
 Terminating at diagram limit
 CALCULATED    68 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE: tcex31c.POLY3
 CPU time for mapping          1  seconds
POLY_3: @@ Add the A2/L1_2 line
POLY_3: read tcex31c
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:
POLY_3: s-c x(b)=.15 t=110
   ... the command in full is SET_CONDITION
POLY_3: s-a-s f
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    38 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
```

```
  ... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =     1, label A0  , database: User dat

Conditions:
T=110, P=1E5, N=1., X(B)=0.15
DEGREES OF FREEDOM 0

Temperature    110.00 K (  -163.15 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
Total Gibbs energy -1.66707E+03,  Enthalpy -1.39975E+03,  Volume  0.00000E+00

Component               Moles       M-Fraction  Activity   Potential  Ref.stat
A                       8.5000E-01  8.5000E-01 7.3635E-01 -2.7991E+02 SER
B                       1.5000E-01  1.5000E-01 2.9909E-05 -9.5277E+03 SER

LRO#1                        Status ENTERED     Driving force  0.0000E+00
Moles 7.2552E-01, Mass 7.2552E+00, Volume fraction 0.0000E+00  Mole fractions:
A  8.40743E-01  B  1.59257E-01
Constitution:
Sublattice  1,  Number of sites  2.5000E-01
A  9.74694E-01  B  2.53056E-02
Sublattice  2,  Number of sites  2.5000E-01
A  9.74694E-01  B  2.53056E-02
Sublattice  3,  Number of sites  2.5000E-01
A  9.74694E-01  B  2.53056E-02
Sublattice  4,  Number of sites  2.5000E-01
B  5.61112E-01  A  4.38888E-01

LRO#2                        Status ENTERED     Driving force -8.1131E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
A  8.60606E-01  B  1.39394E-01
Constitution:
Sublattice  1,  Number of sites  2.5000E-01
A  8.60606E-01  B  1.39394E-01
Sublattice  2,  Number of sites  2.5000E-01
A  8.60606E-01  B  1.39394E-01
Sublattice  3,  Number of sites  2.5000E-01
A  8.60606E-01  B  1.39394E-01
Sublattice  4,  Number of sites  2.5000E-01
A  8.60606E-01  B  1.39394E-01

LRO#3                        Status ENTERED     Driving force  0.0000E+00
Moles 2.7448E-01, Mass 2.7448E+00, Volume fraction 0.0000E+00  Mole fractions:
A  8.74469E-01  B  1.25531E-01
Constitution:
Sublattice  1,  Number of sites  2.5000E-01
A  8.74469E-01  B  1.25531E-01
Sublattice  2,  Number of sites  2.5000E-01
A  8.74469E-01  B  1.25531E-01
Sublattice  3,  Number of sites  2.5000E-01
A  8.74469E-01  B  1.25531E-01
Sublattice  4,  Number of sites  2.5000E-01
A  8.74469E-01  B  1.25531E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: map -
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   1.593E-01  1.100E+02
    LRO#1
  ** LRO#3
*** SORRY CANNOT CONTINUE ***    4
```

```
 CALCULATED    59 EQUILIBRIA

 Phase region boundary   2 at:   1.593E-01  1.100E+02
     LRO#1
  ** LRO#3
 Terminating at diagram limit
 CALCULATED    69 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE: tcex31c.POLY3
 CPU time for mapping           1  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-s x n 0 .5
   ... the command in full is SET_SCALING_STATUS
POST: @@ Usually some 2nd order lines also appear
POST: set-title example 31b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: a-e-d y tcex31 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: set-title example 31c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: ba
   ... the command in full is BACK
POLY_3: read tcex31c
   ... the command in full is READ_WORKSPACES
POLY_3: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: @@ Now we will add a reciprocal parameter to LRO which describes
GES: @@ the SRO contribution.  The default value of this is
GES: @@ the bond energy.  One can have 3 different such parameters
GES: @@ depending on if one is at 25%B, 50%B or 75%B.  Here we just take the
GES: @@ same value.
GES:
GES: e-sym f GSROAA,,UIJ;,,,,,
   ... the command in full is ENTER_SYMBOL
GES: e-sym f GSROAB,,UIJ;,,,,,
   ... the command in full is ENTER_SYMBOL
GES: e-sym f GSROBB,,UIJ;,,,,,
   ... the command in full is ENTER_SYMBOL
GES:
GES: e-par l(lro,a,b:a,b:*:*),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,A,B:A,B:*:*;0)
GES: e-par l(lro,a,b:*:a,b:*),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,A,B:*:A,B:*;0)
GES: e-par l(lro,a,b:*:*:a,b),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,A,B:*:*:A,B;0)
GES: e-par l(lro,*:a,b:a,b:*),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,*:A,B:A,B:*;0)
GES: e-par l(lro,*:a,b:*:a,b),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,*:A,B:*:A,B;0)
GES: e-par l(lro,*:*:a,b:a,b),,GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(LRO,*:*:A,B:A,B;0)
GES: l-p-d lro
   ... the command in full is LIST_PHASE_DATA
```

```
 LRO
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: A,B : A,B : A,B : A,B

      G(LRO,A:A:A:A;0) = 0.0
      G(LRO,B:A:A:A;0) = +GA3B1
      G(LRO,A:B:A:A;0) = +GA3B1
      G(LRO,B:B:A:A;0) = +GA2B2
      G(LRO,A:A:B:A;0) = +GA3B1
      G(LRO,B:A:B:A;0) = +GA2B2
      G(LRO,A:B:B:A;0) = +GA2B2
      G(LRO,B:B:B:A;0) = +GA1B3
      G(LRO,A:A:A:B;0) = +GA3B1
      G(LRO,B:A:A:B;0) = +GA2B2
      G(LRO,A:B:A:B;0) = +GA2B2
      G(LRO,B:B:A:B;0) = +GA1B3
      G(LRO,A:A:B:B;0) = +GA2B2
      G(LRO,B:A:B:B;0) = +GA1B3
      G(LRO,A:B:B:B;0) = +GA1B3
      G(LRO,B:B:B:B;0) = 0.0
      L(LRO,A,B:A,B:*:*;0) = +GSROAB
      L(LRO,A,B:*:A,B:*;0) = +GSROAB
      L(LRO,A,B:*:*:A,B;0) = +GSROAB
      L(LRO,*:A,B:A,B:*;0) = +GSROAB
      L(LRO,*:A,B:*:A,B;0) = +GSROAB
      L(LRO,*:*:A,B:A,B;0) = +GSROAB
GES:
GES: @?<Hit_return_to_continue>
GES: @@ These reciprocal parameters do not give any contribution to the
GES: @@ disordered state as the contribution from the ordered phase is zero there.
GES: @@ But it is in the disordered state that the sro contribution
GES: @@ to the Gibbs energy is most important.  We must add regular solution
GES: @@ parameters to the FCC phase giving the same contribution.  These can
GES: @@ be derived by setting all site-fractions for the same element equal,
GES: @@ i.e. the disordered state.
GES: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3+
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;0)
&                          0.375*GSROAA+0.75*GSROAB+0.375*GSROBB;,,,,,
GES: e-par l(fcc,a,b;1),,2*GA3B1-2*GA1B3+0.75*GSROAA-0.75*GSROBB;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;1)
GES: e-par l(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB;,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;2)
GES: e-par l(fcc,a,b;3),,-0.75*GSROAA+0.75*GSROBB;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;3)
GES: e-par l(fcc,a,b;4),,-0.375*GSROAA+0.75*GSROAB-0.375*GSROBB;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;4)
GES: l-p-d fcc
   ... the command in full is LIST_PHASE_DATA

 FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF LRO
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
      G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
      L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3+.375*GSROAA+.75*GSROAB
           +.375*GSROBB
      L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3+.75*GSROAA-.75*GSROBB
      L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB
      L(FCC_A1,A,B;3) = -.75*GSROAA+.75*GSROBB
      L(FCC_A1,A,B;4) = -.375*GSROAA+.75*GSROAB-.375*GSROBB
GES:
GES: @?<Hit_return_to_continue>
GES: ba
   ... the command in full is BACK
```

```
POLY_3: c-st p lro#3=e 0
   ... the command in full is CHANGE_STATUS
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=70, P=1E5, N=1., X(B)=0.33
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: s-c t=40
   ... the command in full is SET_CONDITION
POLY_3: s-a-s f
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    27 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=40, P=1E5, N=1., X(B)=0.33
 DEGREES OF FREEDOM 0

 Temperature     40.00 K (  -233.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -2.81177E+03,  Enthalpy -2.73484E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.7000E-01  6.7000E-01 5.5303E-03 -1.7286E+03 SER
 B                       3.3000E-01  3.3000E-01 2.8612E-07 -5.0109E+03 SER

 LRO#1                        Status ENTERED     Driving force  0.0000E+00
 Moles 9.1974E-01, Mass 9.1974E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.79151E-01  B  3.20849E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  3,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99993E-01  A  6.81574E-06

 LRO#2                        Status ENTERED     Driving force -3.8166E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.26318E-01  B  3.73682E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01

 LRO#3                        Status ENTERED     Driving force  0.0000E+00
 Moles 8.0263E-02, Mass 8.0263E-01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.65144E-01  B  4.34856E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.99996E-01  B  4.15407E-06
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.99996E-01  B  4.15407E-06
 Sublattice  3,  Number of sites  2.5000E-01
 B  8.69708E-01  A  1.30292E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  8.69708E-01  A  1.30292E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: save tcex31d y
```

```
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3: map -
 Version R mapping is selected

 Organizing start points

 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   3.208E-01  4.000E+01
     LRO#1
  ** LRO#3
 MAPPING TERMINATED 1
 CALCULATED    30 EQUILIBRIA

 Phase region boundary   2 at:   3.208E-01  4.000E+01
     LRO#1
  ** LRO#3
 CALCULATED    22 EQUILIBRIA

 Phase region boundary   2 at:   3.685E-01  7.734E+01
     LRO#1
     LRO#2
  ** LRO#3

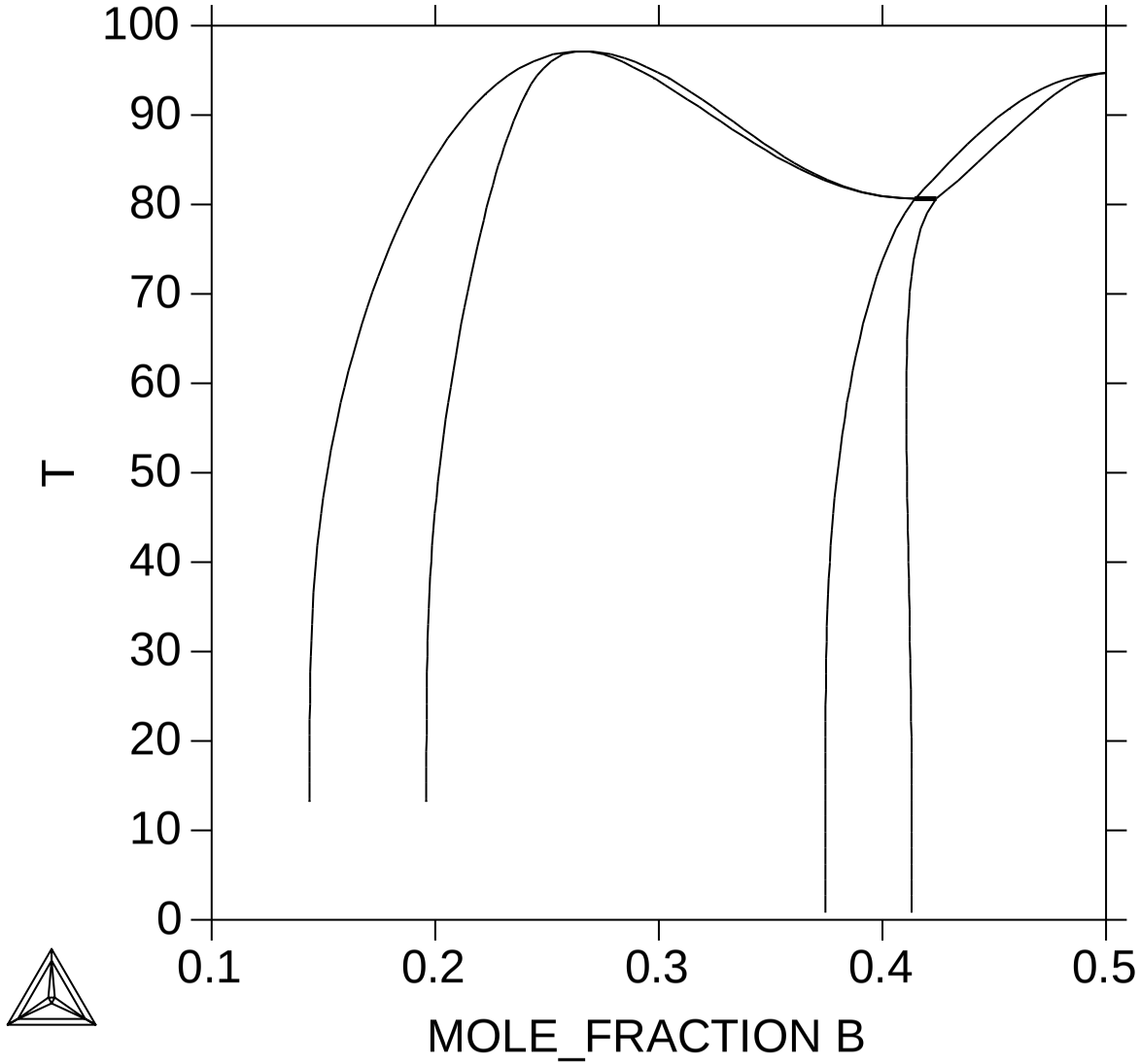
 Phase region boundary   2 at:   4.193E-01  7.734E+01
  ** LRO#2
     LRO#3
 Terminating at diagram limit
 CALCULATED    23 EQUILIBRIA

 Phase region boundary   2 at:   3.685E-01  7.734E+01
     LRO#1
  ** LRO#2
 CALCULATED   100 EQUILIBRA, CONTINUING
 Terminating at known equilibrium
 *** LAST BUFFER SAVED ON FILE: tcex31d.POLY3
 CPU time for mapping           2  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

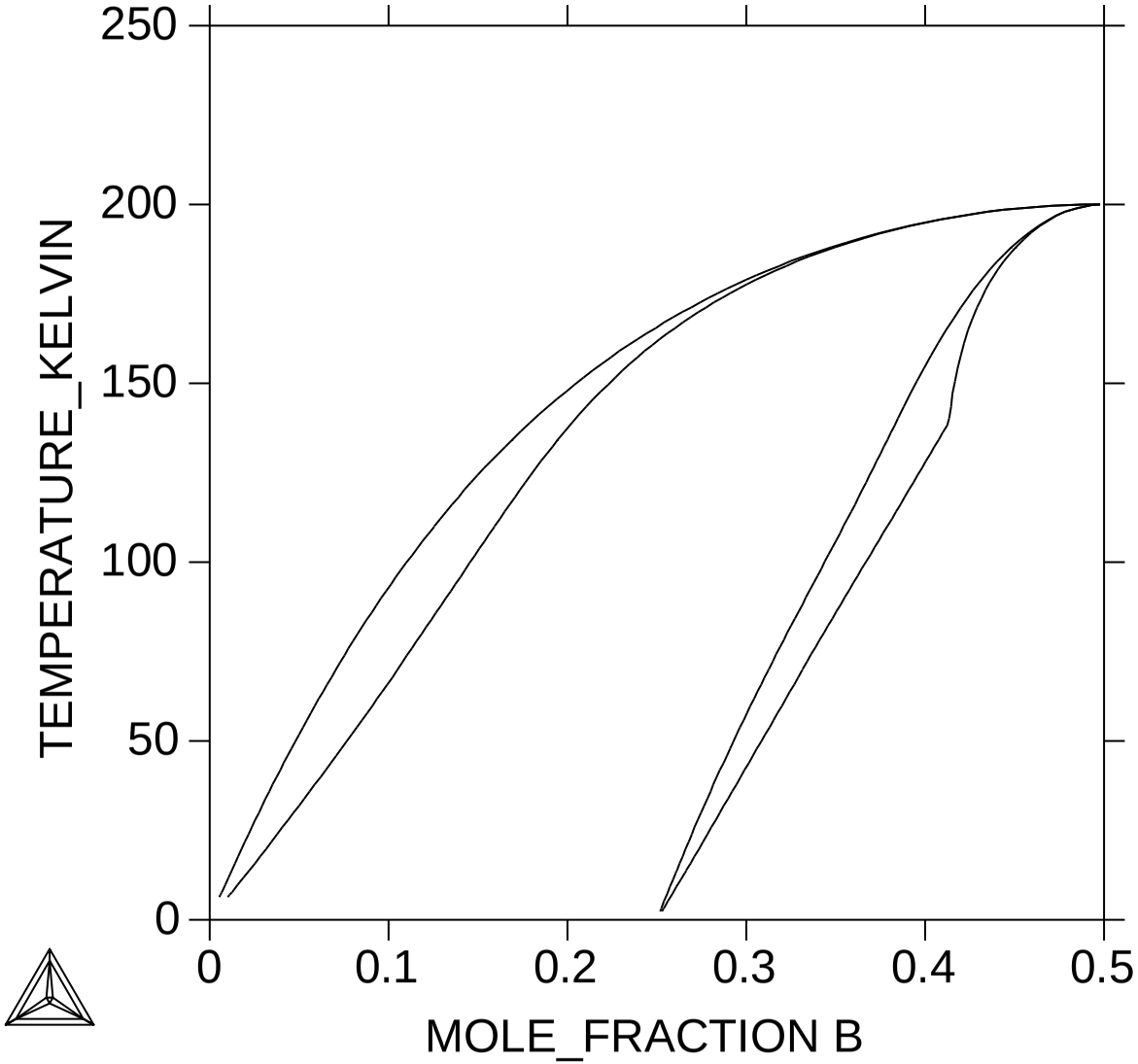
 Setting automatic diagram axis

POST: set-title example 31d
POST: s-s y n
   ... the command in full is SET_SCALING_STATUS
MIN VALUE : 0 100
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: a-e-d y tcex31 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-title example 31e
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
PLOTFILE : /gs/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           8  seconds
```

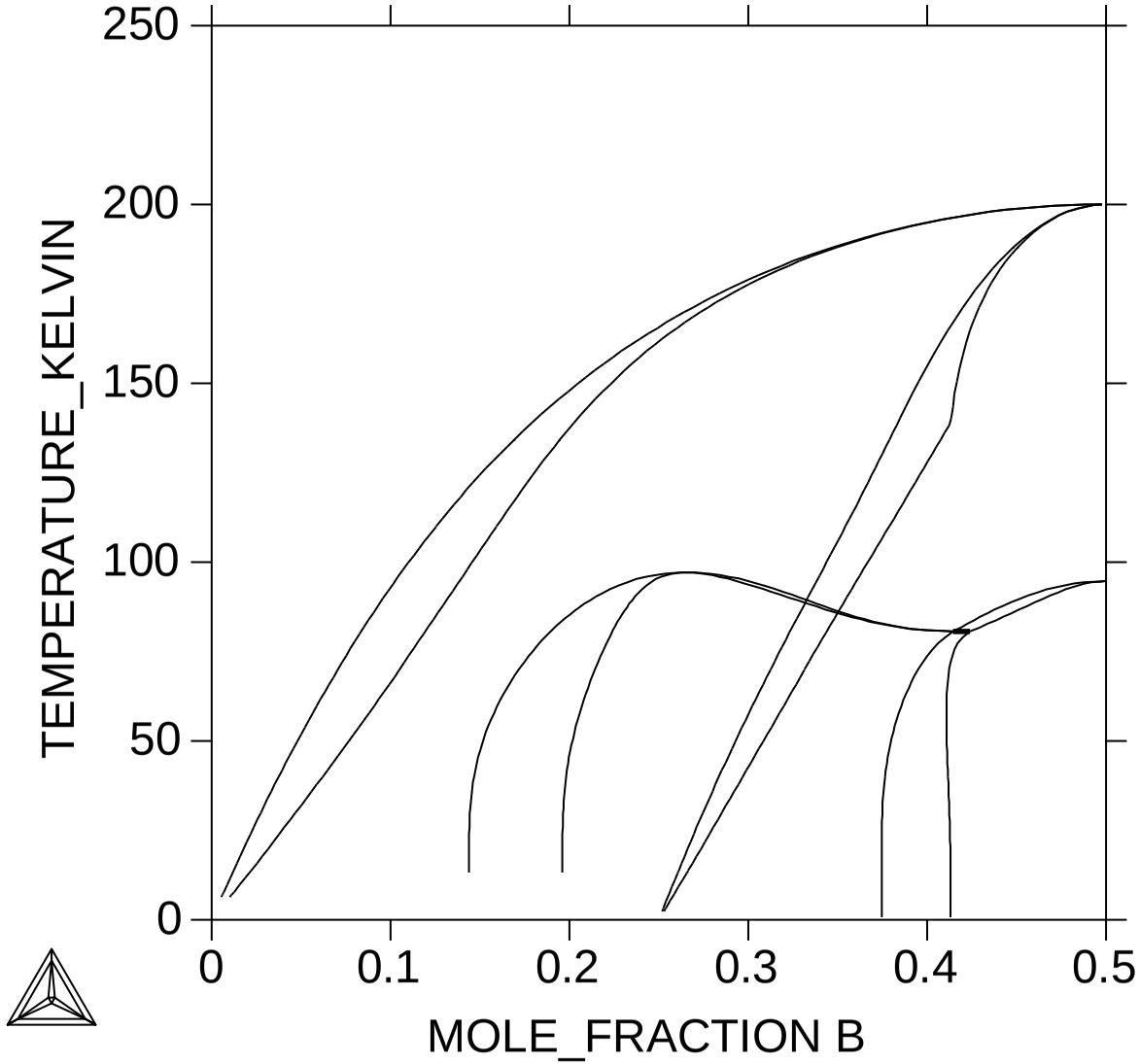
THERMO-CALC (2009.04.15:03.07) :example 31a
DATABASE:User data 2009. 4.15
P=1E5, N=1.;



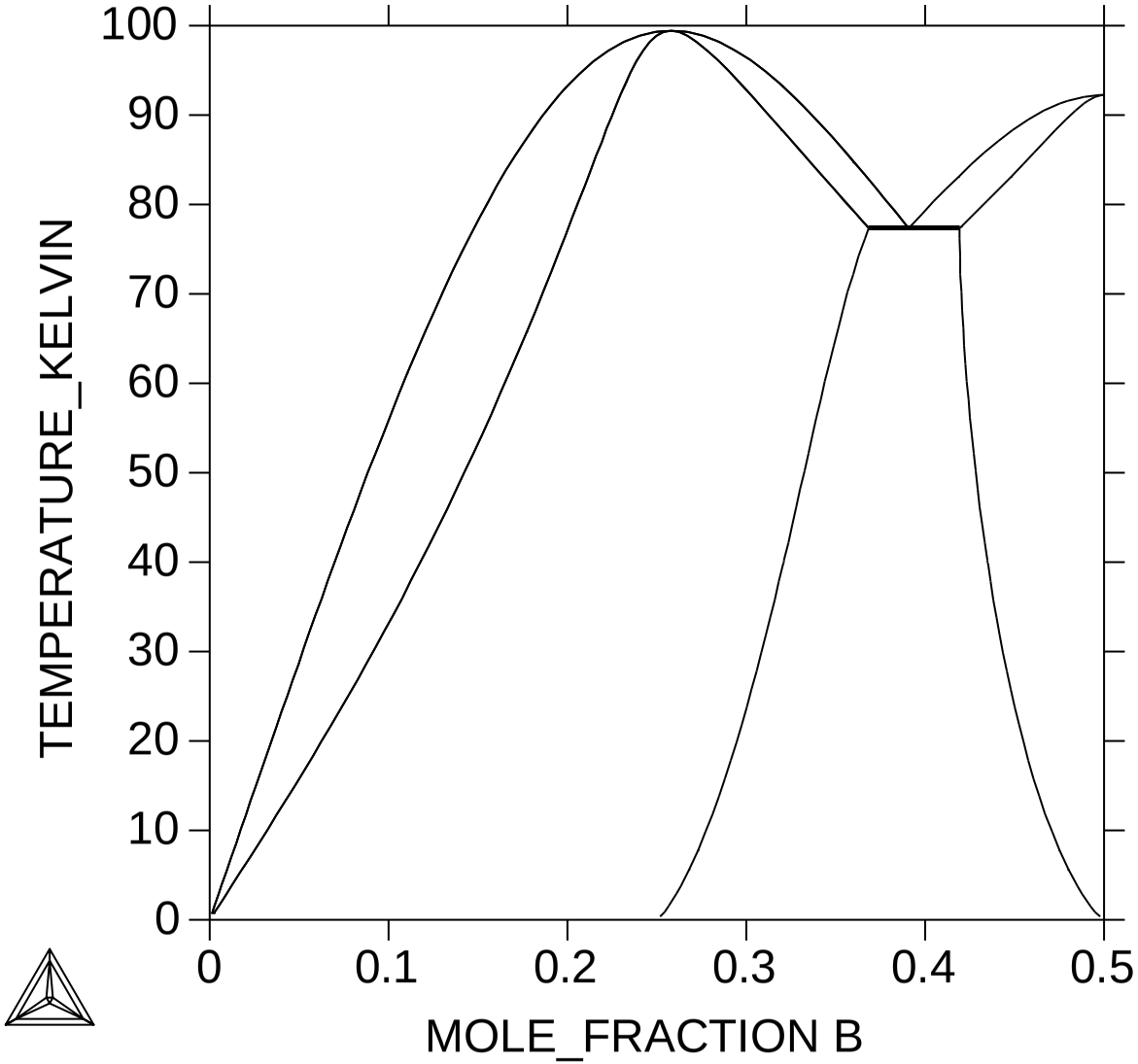
THERMO-CALC (2009.04.15:03.07) :example 31b
DATABASE:User data 2009. 4.15
P=1E5, N=1.;



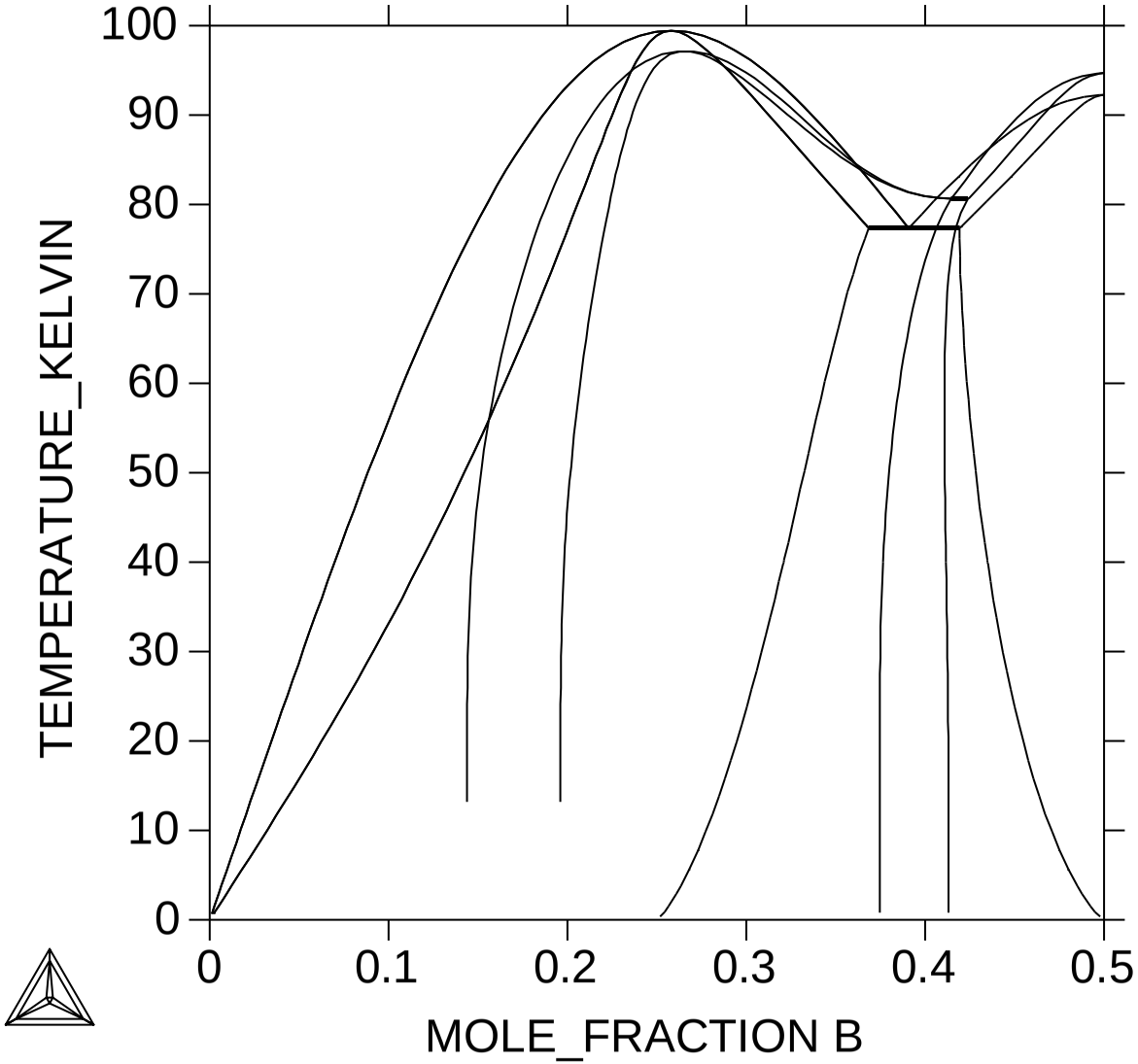
THERMO-CALC (2009.04.15:03.07) :example 31c
DATABASE:User data 2009. 4.15
P=1E5, N=1.;



THERMO-CALC (2009.04.15:03.07) :example 31d
DATABASE:User data 2009. 4.15
P=1E5, N=1.;



THERMO-CALC (2009.04.15:03.07) :example 31e
DATABASE:User data 2009. 4.15
P=1E5, N=1.;



32

Calculation of oxide layers on steel

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of oxide layers on steel
SYS: @@ and show how to append databases
SYS: @@
SYS: set-log ex32,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw tcfe6
   ... the command in full is SWITCH_DATABASE
TDB_TCFE6: d-sys fe cr c v mn si
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
 V                       MN                      SI
   DEFINED
TDB_TCFE6: rej ph /all
   ... the command in full is REJECT
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    MC_ETA
 KSI_CARBIDE             A1_KAPPA                KAPPA
 Z_PHASE                 FE4N_LP1                FECN_CHI
 SIGMA                   CHI_A12                 LAVES_PHASE_C14
 M3SI                    CR3SI                   FE2SI
 MSI                     M5SI3                   AL4C3
 FE8SI2C                 SIC  REJECTED
TDB_TCFE6: rest ph fcc bcc hcp m23 m7 cem
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  HCP_A3
 M23C6                   M7C3                    CEMENTITE
   RESTORED
TDB_TCFE6: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
                    :
                    :
                    :
  'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'K. Frisk, Calphad, 17 (1993), 335-349; Cr-Mn-N'
  'W. Huang, TRITA-MAC 441 (1990); Fe-Mn-V-C'
```

```
  'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
     (1987); C-CR-FE-W'
  'B.-J. Lee, TRITA-MAC 475 (1991); C-Cr-Fe-V'
  'C. Qiu, Metall. Trans. A, 24A (1993), 2393-2409; Cr-Fe-Mn-N'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, Vol.
     53, pp. 105-125; Molar volumes'
 -OK-
TDB_TCFE6: @@ All oxides from the substance database
TDB_TCFE6: app ssub4
   ... the command in full is APPEND_DATABASE
 Current database: SGTE Substances Database v4

 VA  DEFINED
APP:
APP: d-sys fe cr v si mn o c
   ... the command in full is DEFINE_SYSTEM
 FE                    CR                    V
 SI                    MN                    O
 C  DEFINED
APP: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
   C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      CARBON MONOXIDE <GAS>
      STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
   C1O2<G> T.C.R.A.S. Class: 2
      CARBON DIOXIDE <GAS>
   C1SI1<G> T.C.R.A.S. Class: 5
      SILICON CARBIDE <GAS>
                    :
                    :
                    :
   O2SI1<TRIDYMITE> N.P.L.
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   V1 S.G.T.E. **
      VANADIUM
      Data from SGTE Unary DB
   FE0.947O1<WUSTITE> T.C.R.A.S Class: 5
      WUSTITE. Data provided by T.C.R.A.S. in 2000
 -OK-
APP: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c b(cr)=16 b(v)=.1 b(c)=1 b(mn)=.3 b(si)=.3 t=1073 p=1e5 b=100
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100
 DEGREES OF FREEDOM 1
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ We have atomic oxygen as component, later we will use
POLY_3: @@ the partial pressure of o2 as output. The state variable LNACR is
POLY_3: @@ the chemical potential divided by RT, usual values are between -40 and 0
POLY_3: s-c lnacr(o)=-30
   ... the command in full is SET_CONDITION
POLY_3: s-r-s o gas * 1e5
```

```
   ... the command in full is SET_REFERENCE_STATE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         9655  grid points in            0  s
   167 ITS,  CPU TIME USED   1 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB4

 Conditions:
 B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100,
    LNACR(O)=-30
 DEGREES OF FREEDOM 0

 Temperature   1073.00 K (   799.85 C),  Pressure  1.000000E+05
 Number of moles of components  2.11919E+00,  Mass in grams  1.00000E+02
 Total Gibbs energy -2.20047E+05,  Enthalpy -7.06797E+04,  Volume  1.10012E-05

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       8.3257E-02  1.0000E-02 5.8845E-02 -2.5273E+04 SER
 CR                      3.0772E-01  1.6000E-01 4.8455E-04 -6.8091E+04 SER
 FE                      1.3787E+00  7.6998E-01 4.8658E-03 -4.7512E+04 SER
 MN                      5.4607E-03  3.0000E-03 2.1415E-06 -1.1646E+05 SER
 O                       3.3137E-01  5.3016E-02 9.3576E-14 -2.6764E+05 GAS
 SI                      1.0681E-02  3.0000E-03 3.0562E-11 -2.1600E+05 SER
 V                       1.9631E-03  1.0000E-03 4.9690E-08 -1.5004E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.3776E+00, Mass 7.5678E+01, Volume fraction 8.9758E-01  Mass fractions:
 FE  9.73834E-01  C   4.08855E-03  SI  1.08984E-04  O   0.00000E+00
 CR  2.06433E-02  MN  1.26798E-03  V   5.72698E-05

 CR2O3_S                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.1195E-01, Mass 1.5562E+01, Volume fraction 0.0000E+00  Mass fractions:
 CR  6.84207E-01  C   0.00000E+00  MN  0.00000E+00  V   0.00000E+00
 O   3.15793E-01  SI  0.00000E+00  FE  0.00000E+00

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.9165E-01, Mass 7.8927E+00, Volume fraction 1.0242E-01  Mass fractions:
 CR  4.80188E-01  C   8.74967E-02  MN  2.01892E-03  SI  0.00000E+00
 FE  4.18176E-01  V   1.21208E-02  O   0.00000E+00

 BETA_QUARTZ                 Status ENTERED     Driving force  0.0000E+00
 Moles 2.6027E-02, Mass 5.2128E-01, Volume fraction 0.0000E+00  Mass fractions:
 O   5.32554E-01  C   0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
 SI  4.67446E-01  V   0.00000E+00  FE  0.00000E+00

 TEPHROITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.1984E-02, Mass 3.4575E-01, Volume fraction 0.0000E+00  Mass fractions:
 MN  5.44054E-01  SI  1.39069E-01  V   0.00000E+00  CR  0.00000E+00
 O   3.16878E-01  C   0.00000E+00  FE  0.00000E+00
POLY_3: sh lnacr(o)
   ... the command in full is SHOW_VALUE
 LNACR(O)=-30.
POLY_3: @@ List also the activity of O2
POLY_3: show lnacr(o2,gas)
   ... the command in full is SHOW_VALUE
 LNACR(O2,GAS)=-60.
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@ Vary the normalized chemical potential of oxygen between -20 and -40
POLY_3: s-a-v 1 lnacr(o)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  -40
Max value /1/:  -20
Increment /.5/:  0.25
POLY_3: save tcex32 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  NORMAL
```

```
No initial equilibrium, using default
Step will start from axis value   -30.0000
Global calculation of initial equilibrium . impossible due to conditions.
POLY has calculated initial equilibrium
Global test of initial equilibrium

Phase Region from   -30.0000     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1#1
    M7C3
    TEPHROITE
Global check of adding phase at -2.96509E+01
Calculated     4 equilibria

Phase Region from   -29.6509     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1#1
    M7C3
    TEPHROITE
Global check of removing phase at -2.95537E+01
Calculated     3 equilibria

Phase Region from   -29.5537     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1#1
    TEPHROITE
Global check of adding phase at -2.90340E+01
Backtracking to find phase change for FCC_A1#2
Global check of adding phase at -2.95372E+01
Calculated     4 equilibria

Phase Region from   -29.5372     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1#1
    FCC_A1#2
    TEPHROITE
Global check of adding phase at -2.82626E+01
Calculated     8 equilibria

      :
      :
      :

Phase Region from   -31.0652     for:
    BCC_A2
    BETA_QUARTZ
    CR2O3_S
    M23C6
    M7C3
    TEPHROITE
Global check of removing phase at -3.10728E+01
Calculated     3 equilibria

Phase Region from   -31.0728     for:
    BCC_A2
    BETA_QUARTZ
    M23C6
    M7C3
    TEPHROITE
Global check of removing phase at -3.12947E+01
Calculated     4 equilibria

Phase Region from   -31.2947     for:
    BCC_A2
    M23C6
    M7C3
    TEPHROITE
```

```
 Global check of removing phase at -3.14106E+01
 Calculated     3 equilibria

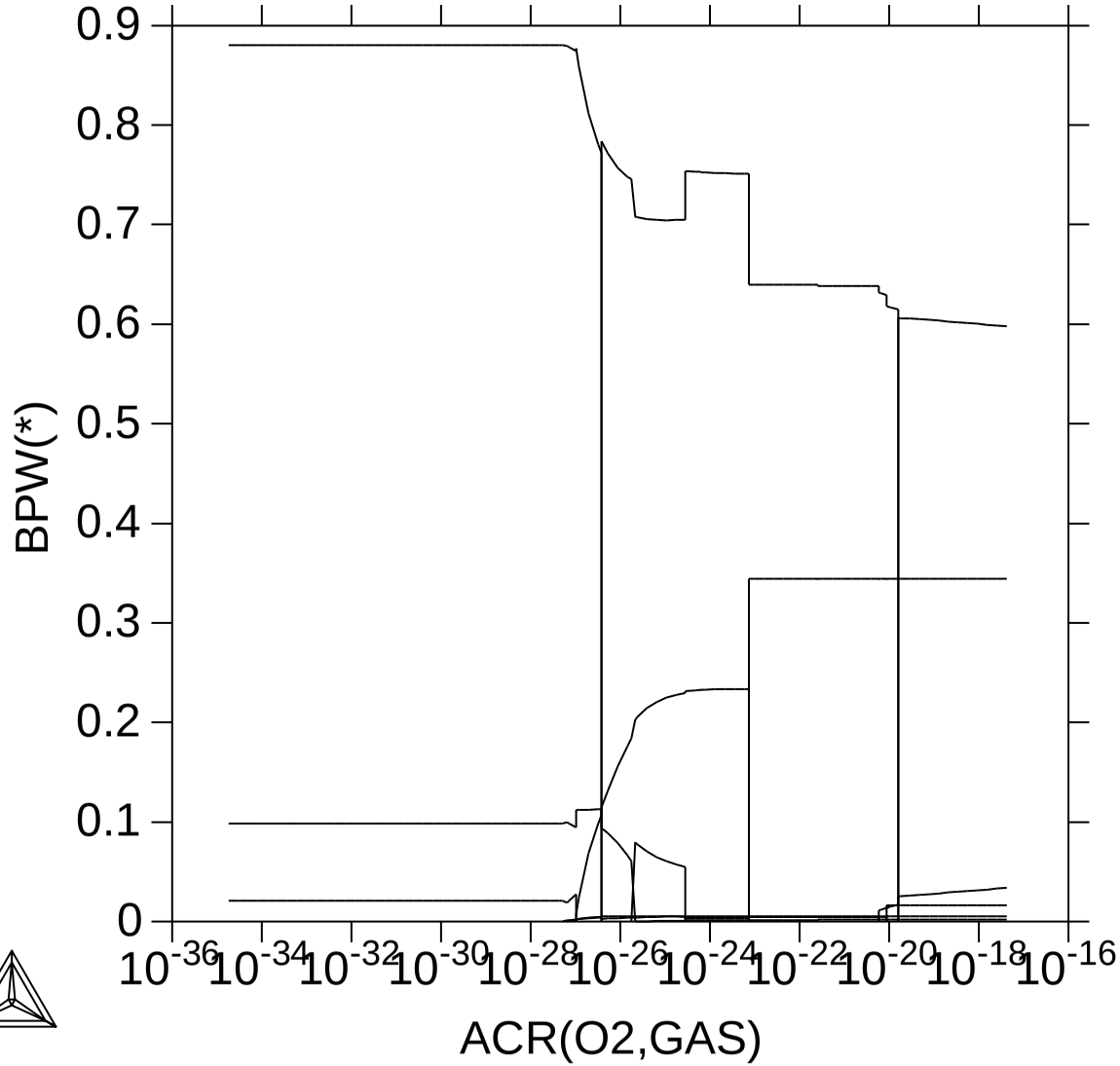
 Phase Region from   -31.4106     for:
     BCC_A2
     M23C6
     M7C3
 Global test at -3.15000E+01 .... OK
 *** Buffer saved on file: tcex32.POLY3
 Global test at -3.32500E+01 .... OK
 Global test at -3.57500E+01 .... OK
 Global test at -3.82500E+01 .... OK
 Terminating at   -40.0000
 Calculated    38 equilibria
 *** Buffer saved on file: tcex32.POLY3
POLY_3:
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

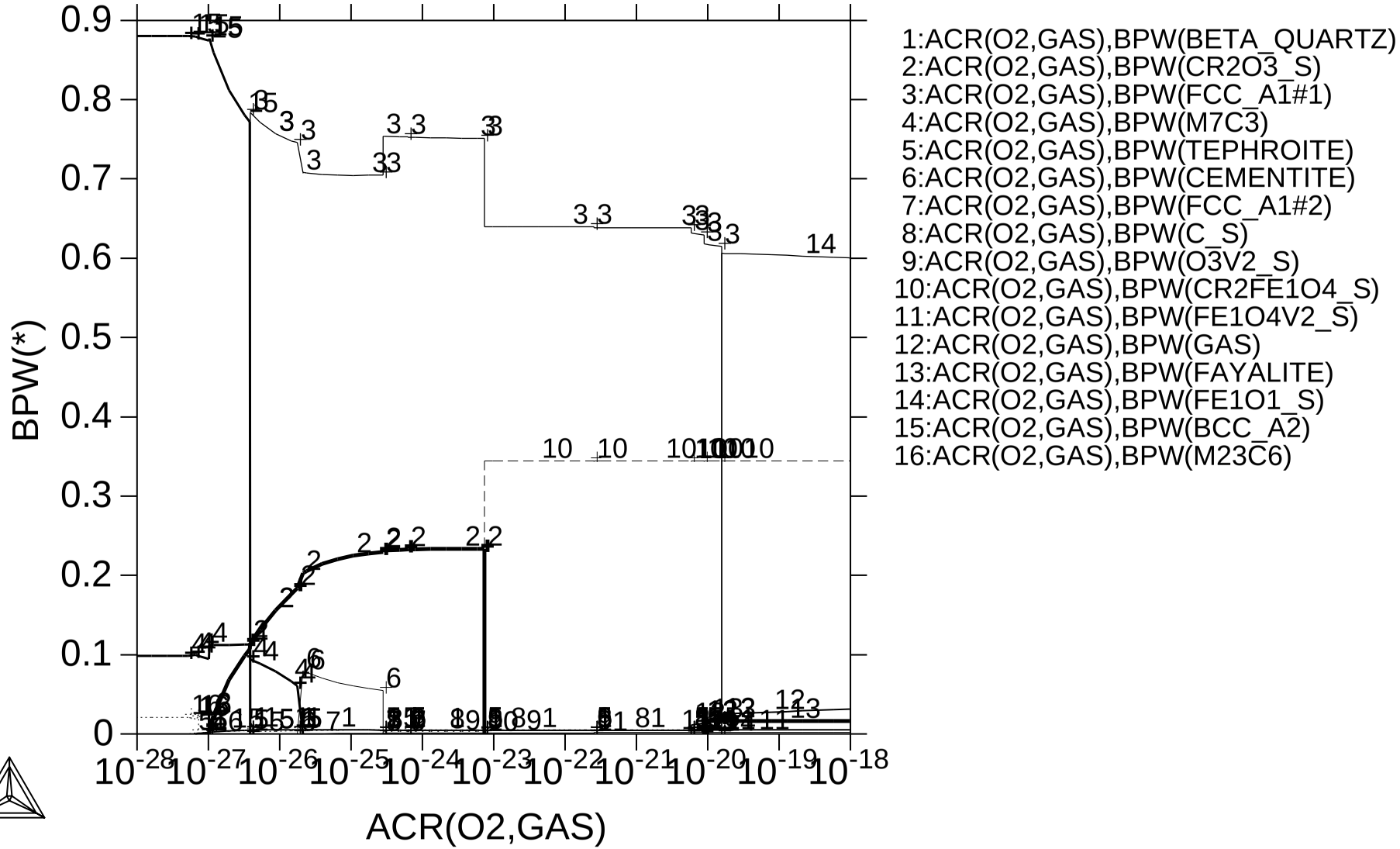
POST: @@ In Thermo-Calc, all lines for metastable phases are dashed in order to
POST: @@ differ from the solid phases. However, in this plot, too many dashed
POST: @@ lines are difficult to read. We can force to always use solid lines.
POST: s-p-o
   ... the command in full is SET_PLOT_OPTIONS
PLOT HEADER /Y/:  y
PLOT LOGO /Y/:  y
PLOT FOOTER /Y/:  y
WHITE-CONTOURED-PS-CHARS /N/:  n
PLOT REMOTE EXPONENT(S) /Y/:  y
PLOT SYMBOLS AT NODE POINTS /0/:
SYMBOL SIZE /.1/:
WRITE CONDITIONS? /Y/:  y
WRITE DATABASE NAME? /Y/:  y
Always initiate POST on re-entering: /Y/:  y
Always solid line: /N/:  y
POST:
POST: s-d-a x acr(o2,gas)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y bpw(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: s-a-ty
   ... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/:  log
POST: set-title example 32a
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-lab f
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s x n 1e-28 1e-18
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 32b
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-a-ty y
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/:  log
POST: s-s y n 1e-4 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 32c
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
```

POST: ***@@ Finally plot how the composition of FCC varies.***
POST: **s-d-a y w(fcc#2,*)**
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *****
POST: **s-s y n 1e-12 1**
... the command in full is SET_SCALING_STATUS
POST: **set-title example 32d**
POST: **pl**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **set-inter**
... the command in full is SET_INTERACTIVE_MODE
POST: CPU time 13 seconds

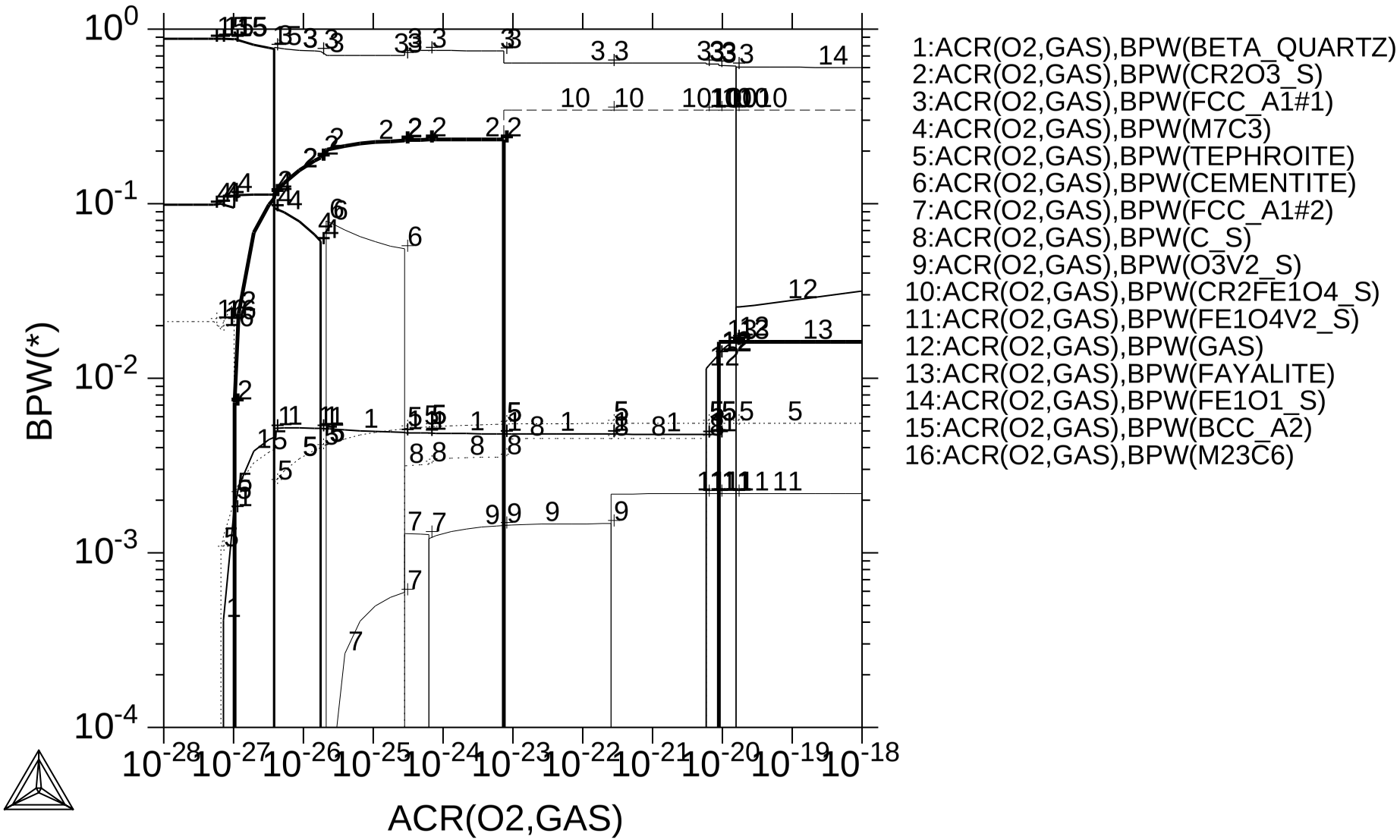
THERMO-CALC (2009.04.15:03.07) :example 32a
DATABASE:SSUB4
B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100.;



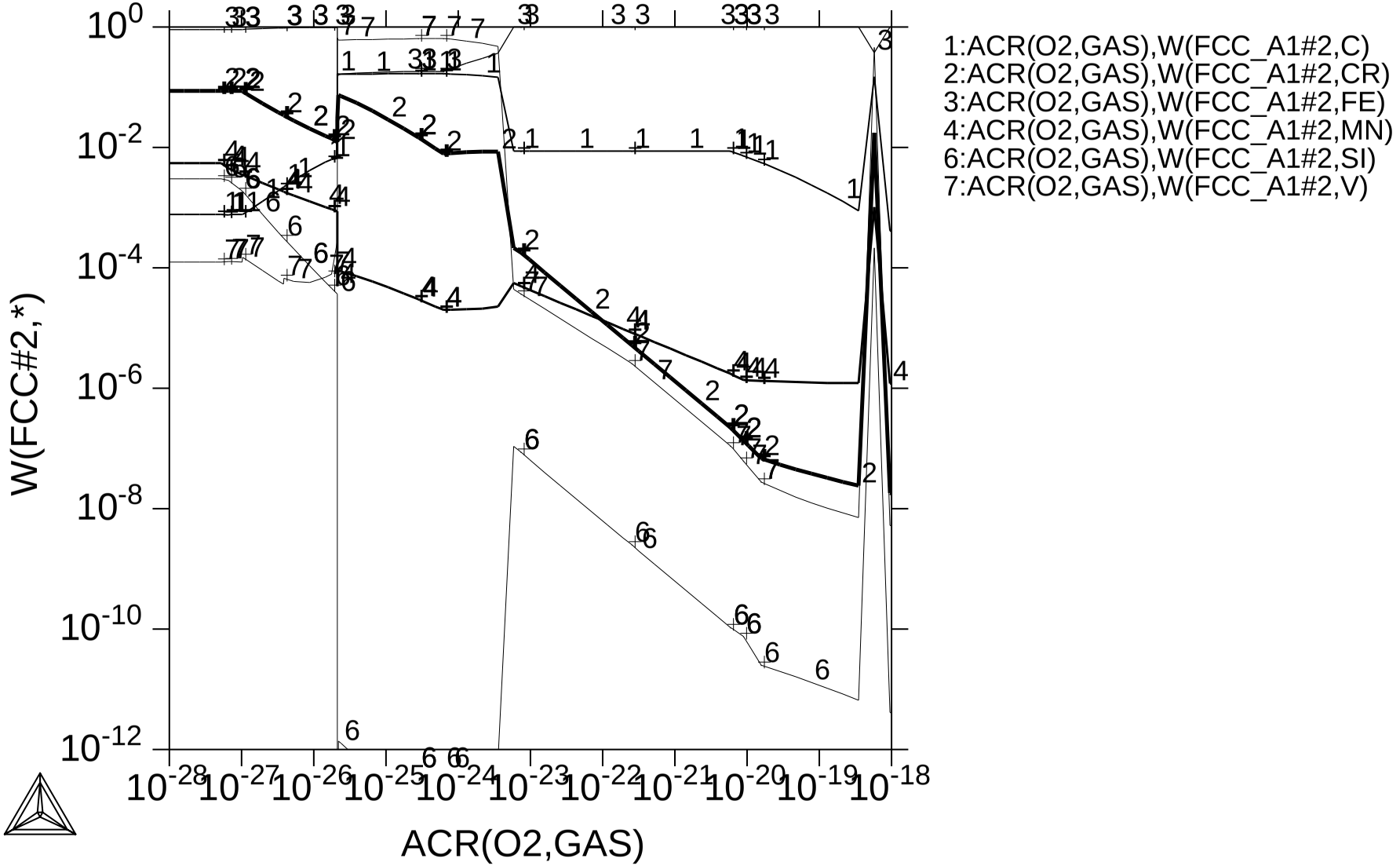
THERMO-CALC (2009.04.15:03.07) :example 32b
DATABASE:SSUB4
B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100.;



THERMO-CALC (2009.04.15:03.07) :example 32c
DATABASE:SSUB4
B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100.;



THERMO-CALC (2009.04.15:03.07) :example 32d
DATABASE:SSUB4
B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100.;



33

Benchmark calculation
an isopleth in the Fe-Cr-C system

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Benchmark calculation for Fe-Cr-C isopleth
SYS: @@
SYS: set-log ex33,,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw PTERN
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN: d-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
   DEFINED
TDB_PTERN: rej ph /all
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  GRAPHITE                SIGMA
 CEMENTITE               M3C2                    M7C3
 M23C6                   V3C2  REJECTED
TDB_PTERN: rest ph liq fcc bcc gra sigma cem m23 m7 m3c2
   ... the command in full is RESTORE
 LIQUID:L                FCC_A1                  BCC_A2
 GRAPHITE                SIGMA                   CEMENTITE
 M23C6                   M7C3                    M3C2
   RESTORED
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
  'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
       C-FE'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
      (1986); CR-FE'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
      Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'
  'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (1986);
      C-CR-FE'
 -OK-
TDB_PTERN: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1200,p=1e5,n=1 w(cr)=.13 w(c)=.01
```

```
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7847  grid points in            1  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: s-a-v 1 w(c) 0 .02
   ... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/:  5E-04
POLY_3: s-a-v 2 t 800 2000
   ... the command in full is SET_AXIS_VARIABLE
Increment /30/:  30
POLY_3: save tcex33 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.400E-03  8.100E+02
     BCC_A2
     M23C6
  ** M7C3
 *** Buffer saved on file: tcex33.POLY3
 Calculated..            2  equilibria
 Terminating at axis limit.
```

```
 Phase region boundary   2 at:   7.432E-03  8.000E+02
    BCC_A2
    M23C6
  ** M7C3
 Calculated.           11  equilibria

 Phase region boundary   3 at:   6.072E-03  1.087E+03
    BCC_A2
  ** FCC_A1#1
    M23C6
  ** M7C3

 Phase region boundary   4 at:   6.072E-03  1.087E+03
    BCC_A2
  ** FCC_A1#1
    M23C6
 Calculated.           13  equilibria

       :
       :
       :

 Phase region boundary  57 at:   1.317E-02  1.687E+03
    LIQUID
  ** FCC_A1#1
 Calculated.           10  equilibria
 Terminating at known equilibrium

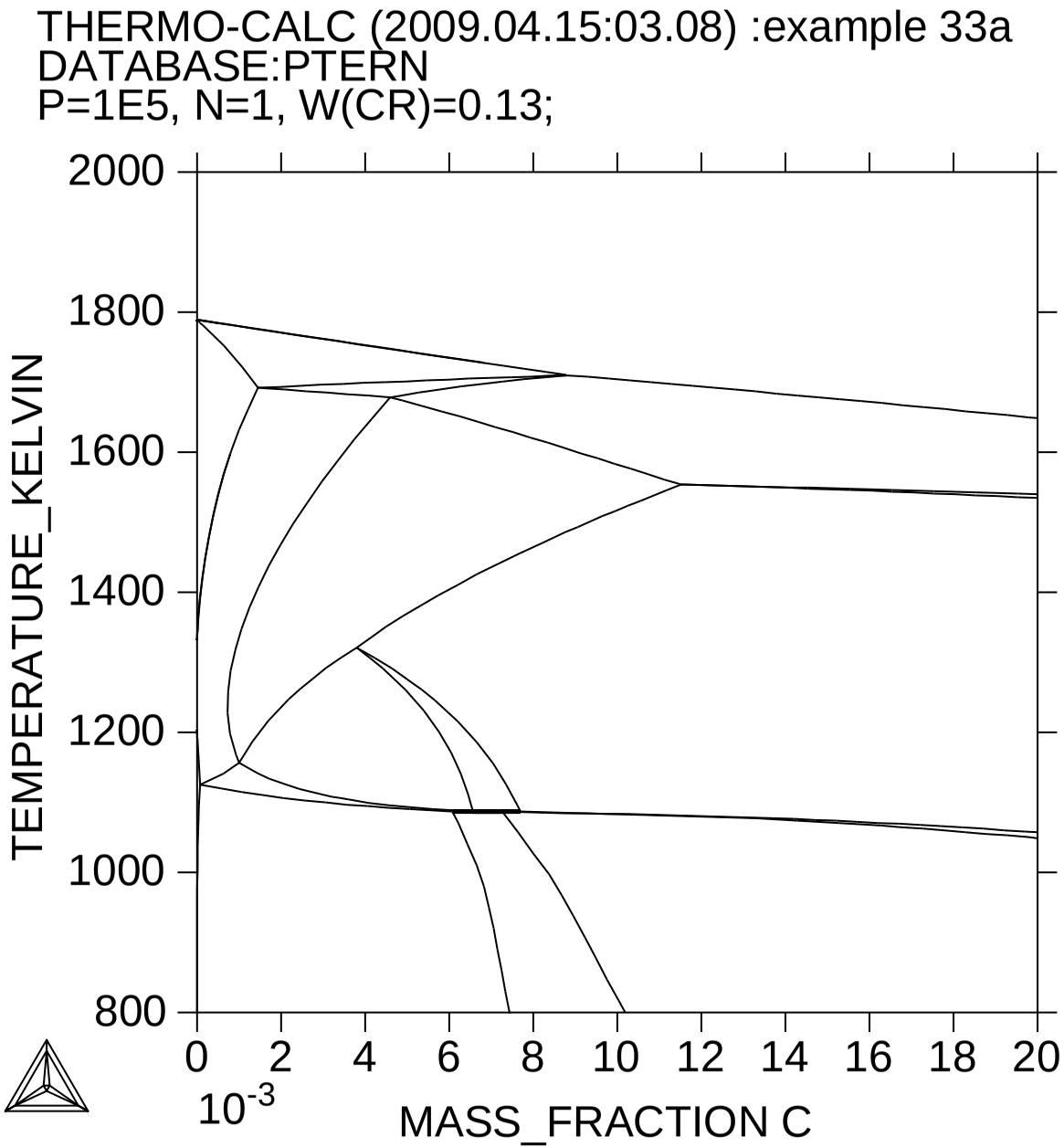
 Phase region boundary  58 at:   1.317E-02  1.687E+03
    LIQUID
  ** FCC_A1#1
 Calculated..           15  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  59 at:   1.950E-02  1.651E+03
    LIQUID
  ** FCC_A1#1
 Calculated.           23  equilibria
 Terminating at known equilibrium

 Phase region boundary  60 at:   1.950E-02  1.651E+03
    LIQUID
  ** FCC_A1#1
 Calculated..            3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: tcex33.POLY3
 CPU time for mapping           9  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST:
POST: set-title example 33a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           10  seconds
```


THERMO-CALC (2009.04.15:03.08) :example 33a
DATABASE:PTERN
P=1E5, N=1, W(CR)=0.13;
2000
1800
1600
1400
1200
1000
800
TEMPERATURE_KELVIN
0
2
4
6
8
10
12
14
16
18
20
10-3
MASS_FRACTION C

34

Calculation of the phase diagram and G curves in the Al-Zn system

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Another example of using the BINARY module
SYS: @@
SYS: go bin
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/:  PBIN
 Current database: TCS Public Binary Alloys TDB v1

 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:  Phase_Diagram
 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
 REINITIATING GES5 .....
 AL                      ZN  DEFINED
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  ALCU_THETA              AL3NI2
 TIAL                    TI3AL                   CUZN_EPS
   REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   91Din 'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, Vol.15,
       No.4, pp.317-425, (1991)'
   MAY-ALZN 'S. an Mey, Zeit. fur Metallkde, 84, (7),
       451-455 (1993), Al-Zn '
 -OK-
 The condition X(ZN)=.1234  created
 The condition T=1319.08  created
 Forcing automatic start values
 Automatic start values will be set
 Start points provided by database
 Version S mapping is selected

 Organizing start points

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   3.640E-01  5.600E+02
  ** FCC_A1#1
     FCC_A1#2
 *** Buffer saved on file: BINARY.POLY3
 Calculated.            2  equilibria

 Phase region boundary   2 at:   3.658E-01  5.504E+02
```

```
 ** FCC_A1#1
    FCC_A1#2
 ** HCP_A3

 Phase region boundary   3 at:   5.626E-01  5.504E+02
    FCC_A1#1
 ** HCP_A3
 Calculated..           13  equilibria
 Terminating at axis limit.

 Phase region boundary   4 at:   7.872E-01  5.504E+02
    FCC_A1#1
 ** HCP_A3
 Calculated.            6  equilibria

       :
       :
       :

 Phase region boundary   6 at:   7.783E-01  6.540E+02
 ** LIQUID
    FCC_A1#1
 Calculated           73  equilibria

 Phase region boundary   7 at:   9.263E-01  6.540E+02
 ** LIQUID
    HCP_A3
 Calculated           17  equilibria

 Phase region boundary   8 at:   3.658E-01  5.504E+02
    FCC_A1#1
 ** FCC_A1#2
 Calculated           27  equilibria

 Phase region boundary   9 at:   3.640E-01  5.600E+02
 ** FCC_A1#1
    FCC_A1#2
 Calculated           28  equilibria
 *** BUFFER SAVED ON FILE: BINARY.POLY3
 CPU time for mapping           0  seconds

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: set-title example 34a
POST: plot
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Now plot a G curve at 573 K!
POST: back
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
SYS: go bin
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: PBIN
 Current database: TCS Public Binary Alloys TDB v1
```

```
 VA                     /-  DEFINED
 IONIC_LIQ:Y            L12_FCC                B2_BCC
 BCC_B2  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:  G
Temperature (C): /1000/:  300
 VA                     /-  DEFINED
 IONIC_LIQ:Y            L12_FCC                B2_BCC
 BCC_B2  REJECTED
 REINITIATING GES5 .....
 AL                     ZN  DEFINED
 LIQUID:L               FCC_A1                 BCC_A2
 HCP_A3                 ALCU_THETA             AL3NI2
 TIAL                   TI3AL                  CUZN_EPS
   REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   91Din 'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, Vol.15,
       No.4, pp.317-425, (1991)'
   MAY-ALZN 'S. an Mey, Zeit. fur Metallkde, 84, (7),
       451-455 (1993), Al-Zn '
 -OK-
 The condition X(ZN)=.1234  created
 Forcing automatic start values
 Automatic start values will be set

 Phase Region from   0.502463     for:
     LIQUID
     FCC_A1#1
     FCC_A1#2
     HCP_A3

 Phase Region from   0.502463     for:
     LIQUID
     FCC_A1#1
     FCC_A1#2
     HCP_A3
 *** Buffer saved on file *** GCURVE.POLY3

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-s y n -500 1500
POST:
POST: set-title example 34b
POST: plot
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Now plot an activity (A) curve at 573 K
POST: back
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y            L12_FCC                B2_BCC
 B2_VACANCY             HIGH_SIGMA             DICTRA_FCC_A1
   REJECTED
SYS: go bin
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y            L12_FCC                B2_BCC
 B2_VACANCY             HIGH_SIGMA             DICTRA_FCC_A1
   REJECTED

 Simple binary phase diagram calculation module
```

```
Database: /TCBIN/: PBIN
 Current database: TCS Public Binary Alloys TDB v1

 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:  A
Temperature (C): /1000/:  300
 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
 REINITIATING GES5 .....
 AL                      ZN  DEFINED
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  ALCU_THETA              AL3NI2
 TIAL                    TI3AL                   CUZN_EPS
   REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   91Din 'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, Vol.15,
       No.4, pp.317-425, (1991)'
   MAY-ALZN 'S. an Mey, Zeit. fur Metallkde, 84, (7),
       451-455 (1993), Al-Zn '
 -OK-
 The condition X(ZN)=.1234  created

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

 Forcing automatic start values
 Automatic start values will be set
 No initial equilibrium, using default
 Step will start from axis value   0.123400
 Global calculation of initial equilibrium ....OK

 Phase Region from   0.123400     for:
     FCC_A1#1
 Global test at  3.23400E-01 .. Backtracking to find phase change for FCC_A1#2
 Global test at  1.48400E-01 .... OK
 Global check of adding phase at  1.70853E-01
 Calculated     5 equilibria

 Phase Region from   0.170853     for:
     FCC_A1#1
     FCC_A1#2
 Global test at  3.48400E-01 .... OK
 Global check of removing phase at  5.51861E-01
 Calculated    19 equilibria

 Phase Region from   0.551861     for:
     FCC_A1#2
 Global check of adding phase at  6.18456E-01
 Calculated     5 equilibria

 Phase Region from   0.618456     for:
     FCC_A1#2
     HCP_A3
 Global test at  7.98400E-01 .... OK
 Global check of removing phase at  9.81102E-01
 Calculated    18 equilibria

 Phase Region from   0.981102     for:
     HCP_A3
```

```
 Terminating at    1.00000
 Calculated     4 equilibria

 Phase Region from   0.123400     for:
     FCC_A1#1
 Terminating at   0.100000E-11
 Calculated     8 equilibria
 *** Buffer saved on file: GCURVE.POLY3

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST:
POST: set-title example 34c
POST: plot
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Now plot a Phase fraction (F) curve for x(zn)=.5.
POST: @@ The miscibility gap can be found now
POST: back
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
SYS: go bin
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/:  PBIN
 Current database: TCS Public Binary Alloys TDB v1

 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:  F
Fraction of: zn /.5/:  .5
 VA                      /-  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 BCC_B2  REJECTED
 REINITIATING GES5 .....
 AL                      ZN  DEFINED
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  ALCU_THETA              AL3NI2
 TIAL                    TI3AL                   CUZN_EPS
   REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   91Din 'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, Vol.15,
       No.4, pp.317-425, (1991)'
   MAY-ALZN 'S. an Mey, Zeit. fur Metallkde, 84, (7),
       451-455 (1993), Al-Zn '
 -OK-
 Forcing automatic start values
 Automatic start values will be set
 No initial equilibrium, using default
 Step will start from axis value    2500.00
 Global calculation of initial equilibrium ....OK
```

```
 Phase Region from    2500.00     for:
     LIQUID
 Global test at  2.42000E+03 .... OK
 Global test at  2.32000E+03 .... OK
 Global test at  2.22000E+03 .... OK
 Global test at  2.12000E+03 .... OK
 Global test at  2.02000E+03 .... OK
 Global test at  1.92000E+03 .... OK
 Global test at  1.82000E+03 .... OK
 Global test at  1.72000E+03 .... OK
 Global test at  1.62000E+03 .... OK
 Global test at  1.52000E+03 .... OK
 Global test at  1.42000E+03 .... OK
 Global test at  1.32000E+03 .... OK
 Global test at  1.22000E+03 .... OK
 Global test at  1.12000E+03 .... OK
 Global test at  1.02000E+03 .... OK
 Global test at  9.20000E+02 .... OK
 Global test at  8.20000E+02 .... OK
 Global check of adding phase at  7.88048E+02
 Calculated   174 equilibria

 Phase Region from    788.048     for:
     LIQUID
     FCC_A1#1
 Global test at  7.26000E+02 .... OK
 Global test at  7.06000E+02 .... OK
 Global check of removing phase at  7.00299E+02
 Calculated    23 equilibria

 Phase Region from    700.299     for:
     FCC_A1#1
 Global test at  6.28000E+02 .... OK
 Global test at  5.28000E+02 .. Backtracking to find phase change for FCC_A1#2
 Global test at  6.18000E+02 .... OK
 Global test at  5.98000E+02 .... OK
 Global check of adding phase at  5.96831E+02
 Calculated    15 equilibria

 Phase Region from    596.831     for:
     FCC_A1#1
     FCC_A1#2
 Global check of adding phase at  5.50386E+02
 Calculated     7 equilibria

 Phase Region from    550.386     for:
     FCC_A1#1
     FCC_A1#2
     HCP_A3
 Calculated     2 equilibria

 Phase Region from    550.386     for:
     FCC_A1#2
     HCP_A3
 Global test at  4.78000E+02 .... OK
 Global test at  3.78000E+02 .... OK
 Terminating at    300.000
 Calculated    29 equilibria
 *** Buffer saved on file: PFCURVE.POLY3

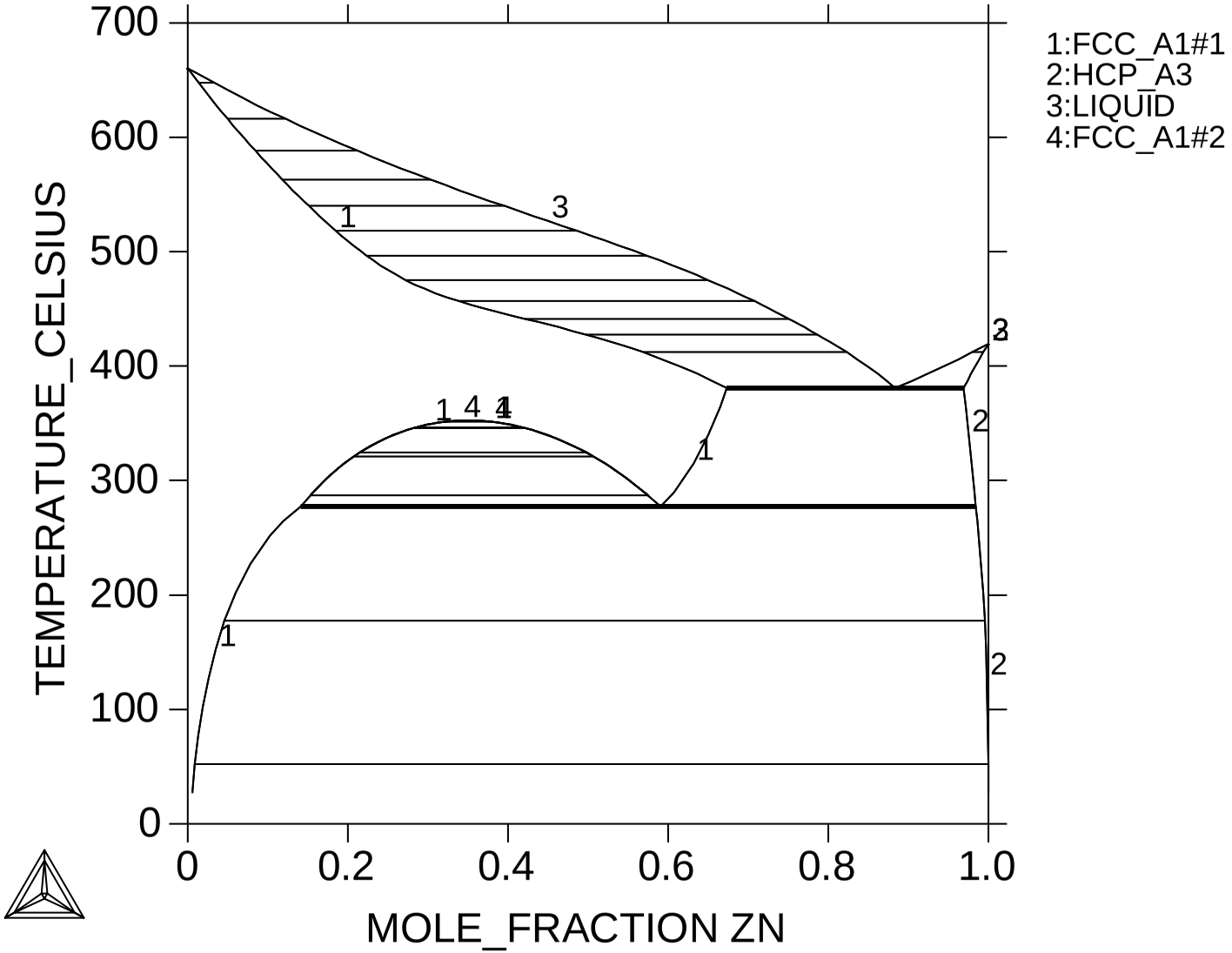
  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

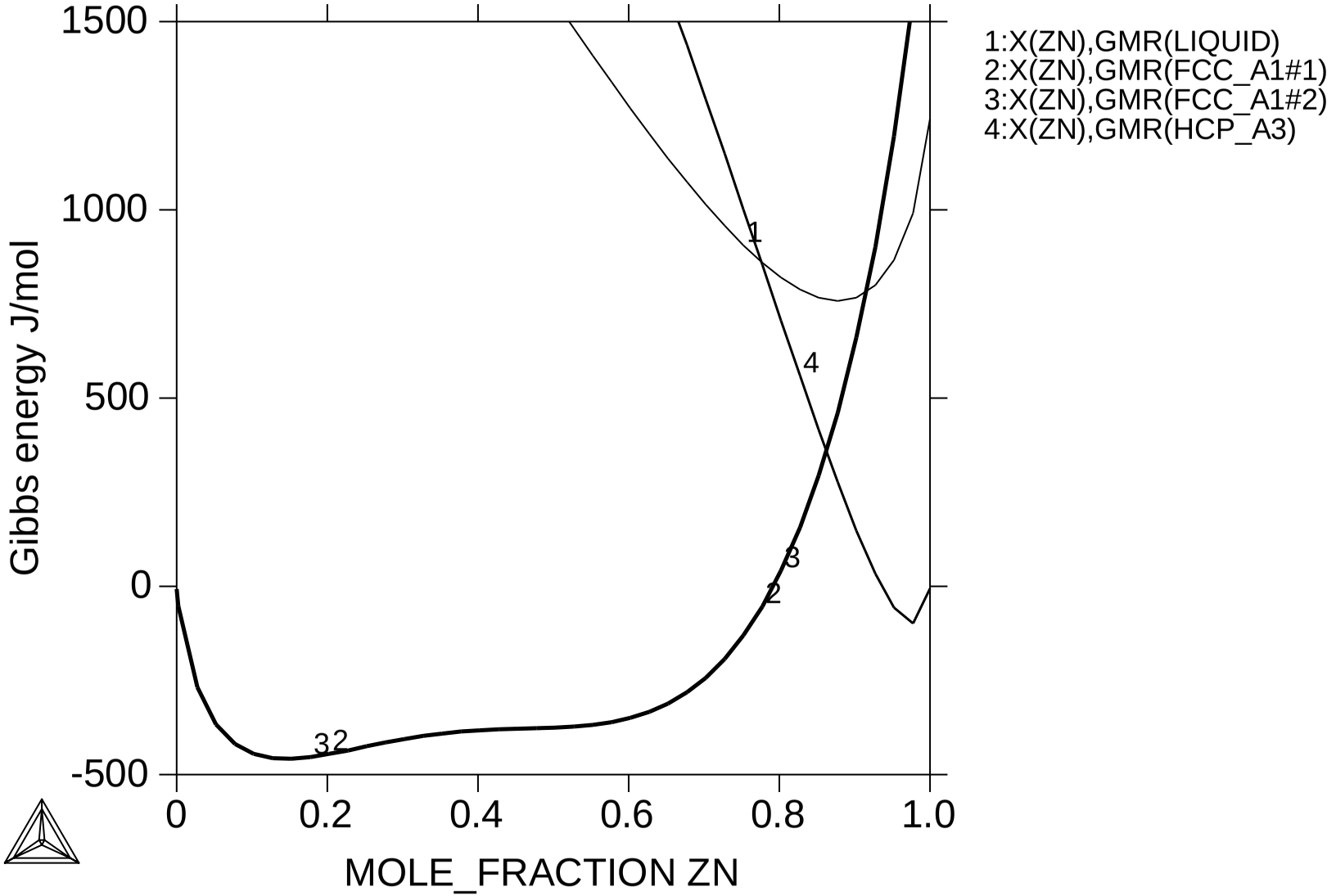
POST:
POST: s-s x n 200 700
POST: set-title example 34d
POST: plot
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
POST: Current database: TCS Steels/Fe-Alloys Database v6
```

```
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
SYS: CPU time            4  seconds
```

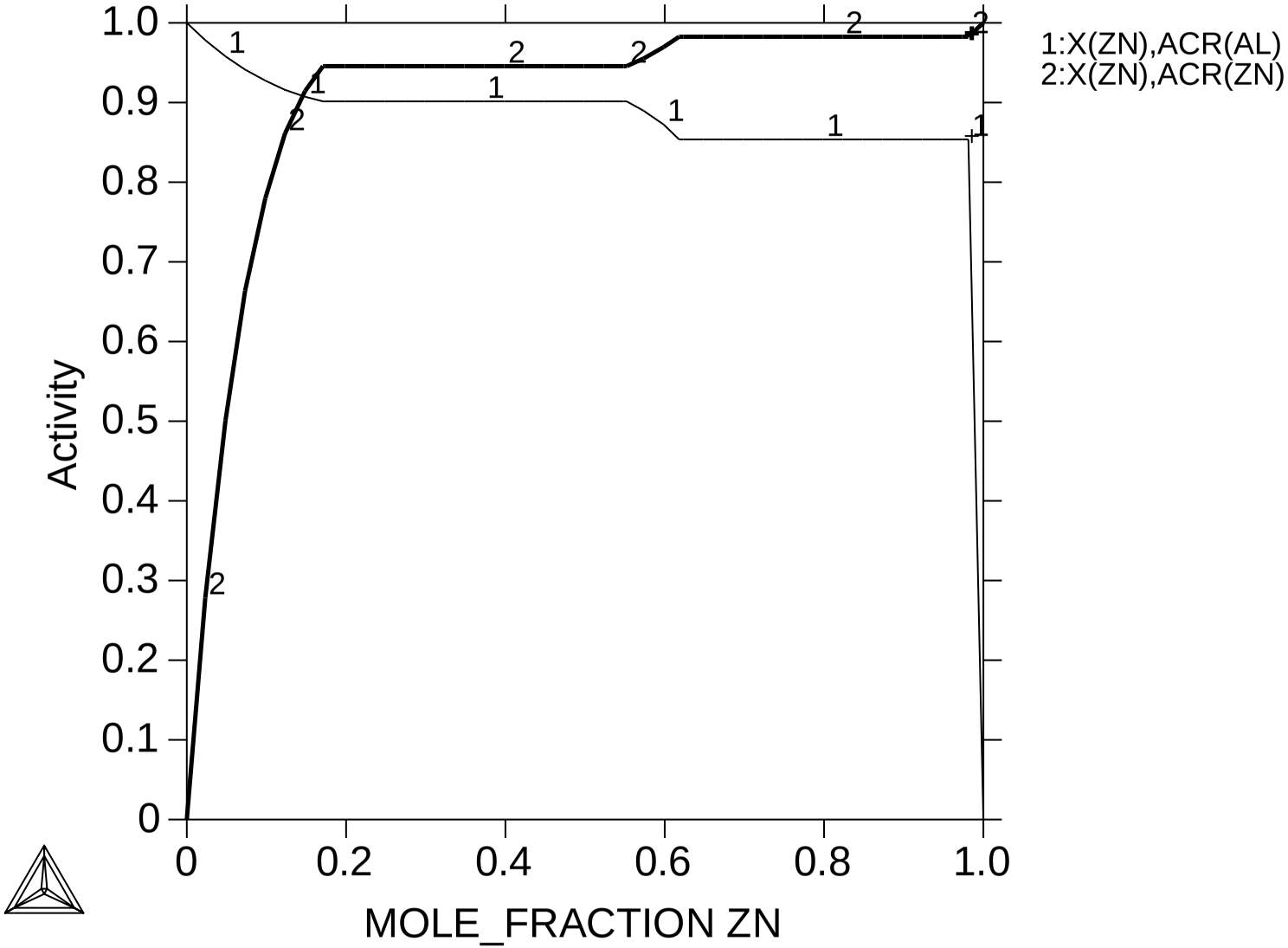
THERMO-CALC (2009.04.15:03.08) :example 34a
DATABASE:PBIN
P=1E5, N=1



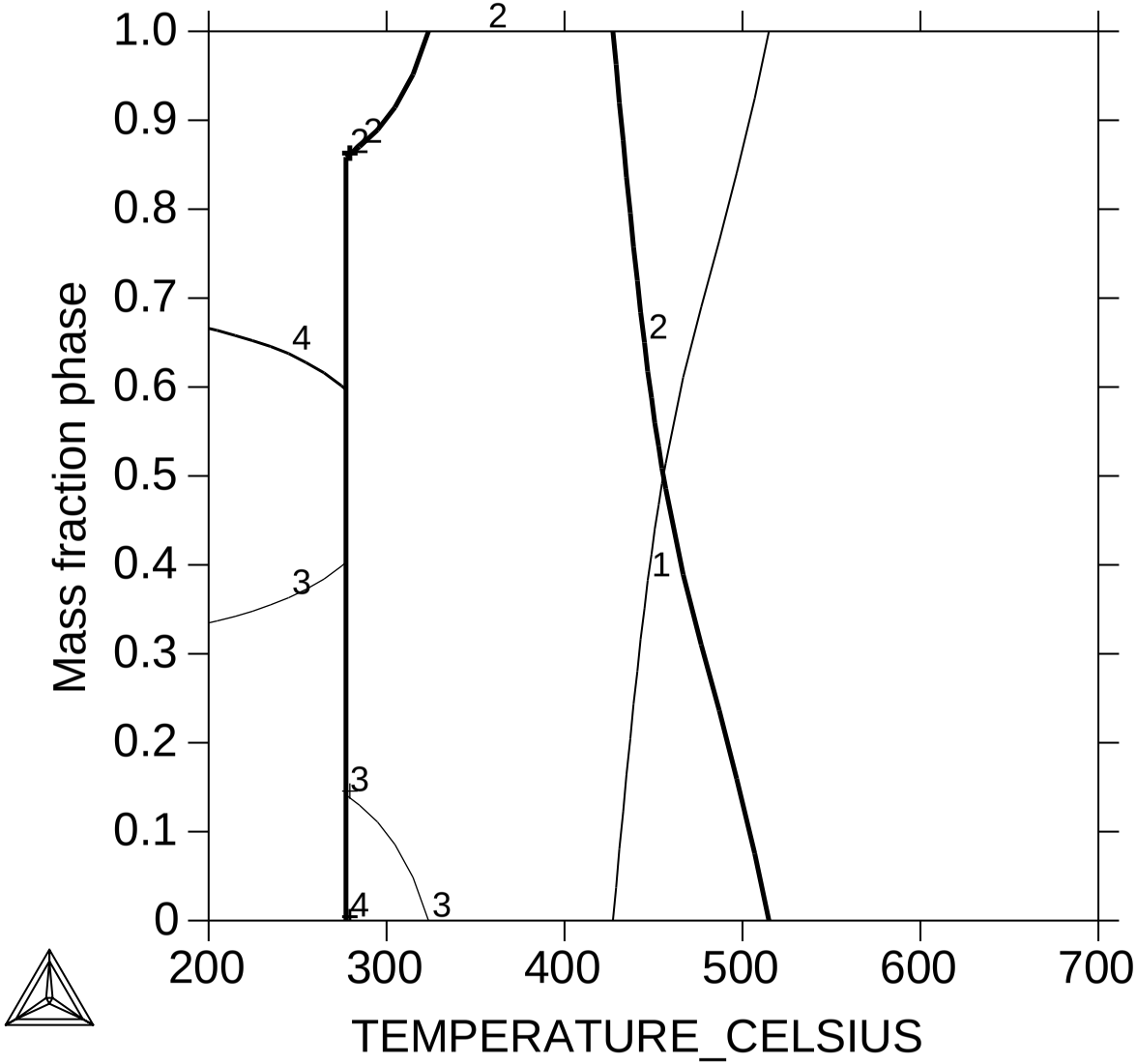
THERMO-CALC (2009.04.15:03.08) :example 34b
DATABASE:PBIN
P=1E5, N=1, T=573.15;



THERMO-CALC (2009.04.15:03.08) :example 34c
DATABASE:PBIN
P=1E5, N=1, T=573.15;



THERMO-CALC (2009.04.15:03.08) :example 34d
DATABASE:PBIN
N=1., P=1E5, X(ZN)=0.5;



1:T-273.15,BPW(LIQUID)
2:T-273.15,BPW(FCC_A1#1)
3:T-273.15,BPW(FCC_A1#2)
4:T-273.15,BPW(HCP_A3)

35

Calculation
of potential diagram

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example of use of the POTENTIAL module
SYS: @@
SYS: go pot
 Simple potential phase diagram calculation module

Database: /POT/: PSUB
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Public Pure Substances TDB v1

 VA  DEFINED
Matrix element: /FE/: FE
First potential species: /S1O2/: S2
Second potential species: /O2/: O2
Temperature: /1000/: 1000
 VA  DEFINED
 REINITIATING GES5 .....
 FE                    S                     O
   DEFINED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous species, stoichiometric solids and
      liquids in the Cu-Fe-H-N-O-S system.'
 -OK-
 This command is DEPRECATED and to be removed in the future!

 Please use ADVANCED_OPTIONS instead of SPECIAL_OPTIONS

 The condition LNACR(S2,GAS)=-140.8589  created
 The condition LNACR(O2,GAS)=-140.8589  created
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         2715  grid points in            0  s
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Working hard
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4

 Phase region boundary   1 at:  -2.173E+01 -1.409E+02
     FE
  ** PYRRHOTITE_S2
 *** Buffer saved on file: POT.POLY3
 Calculated..           81  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:  -2.173E+01 -3.000E+02
     FE
  ** PYRRHOTITE_S2
 Calculated.          128  equilibria

 Phase region boundary   3 at:  -2.173E+01 -4.780E+01
     FE
  ** PYRRHOTITE_S2
```

```
 ** WUSTITE

Phase region boundary   4 at:  -2.173E+01 -4.780E+01
    FE
 ** WUSTITE
Calculated..          141  equilibria
Terminating at axis limit.

      :
      :
      :

Phase region boundary  19 at:  -1.964E+01 -4.554E+01
 ** MAGNETITE
    WUSTITE
Calculated..          142  equilibria
Terminating at axis limit.

Phase region boundary  20 at:  -2.173E+01 -1.409E+02
    FE
 ** PYRRHOTITE_S2
Calculated.           48  equilibria
Terminating at known equilibrium

Phase region boundary  21 at:  -1.409E+02 -4.780E+01
    FE
 ** WUSTITE
Calculated..           81  equilibria
Terminating at known equilibrium
Terminating at axis limit.

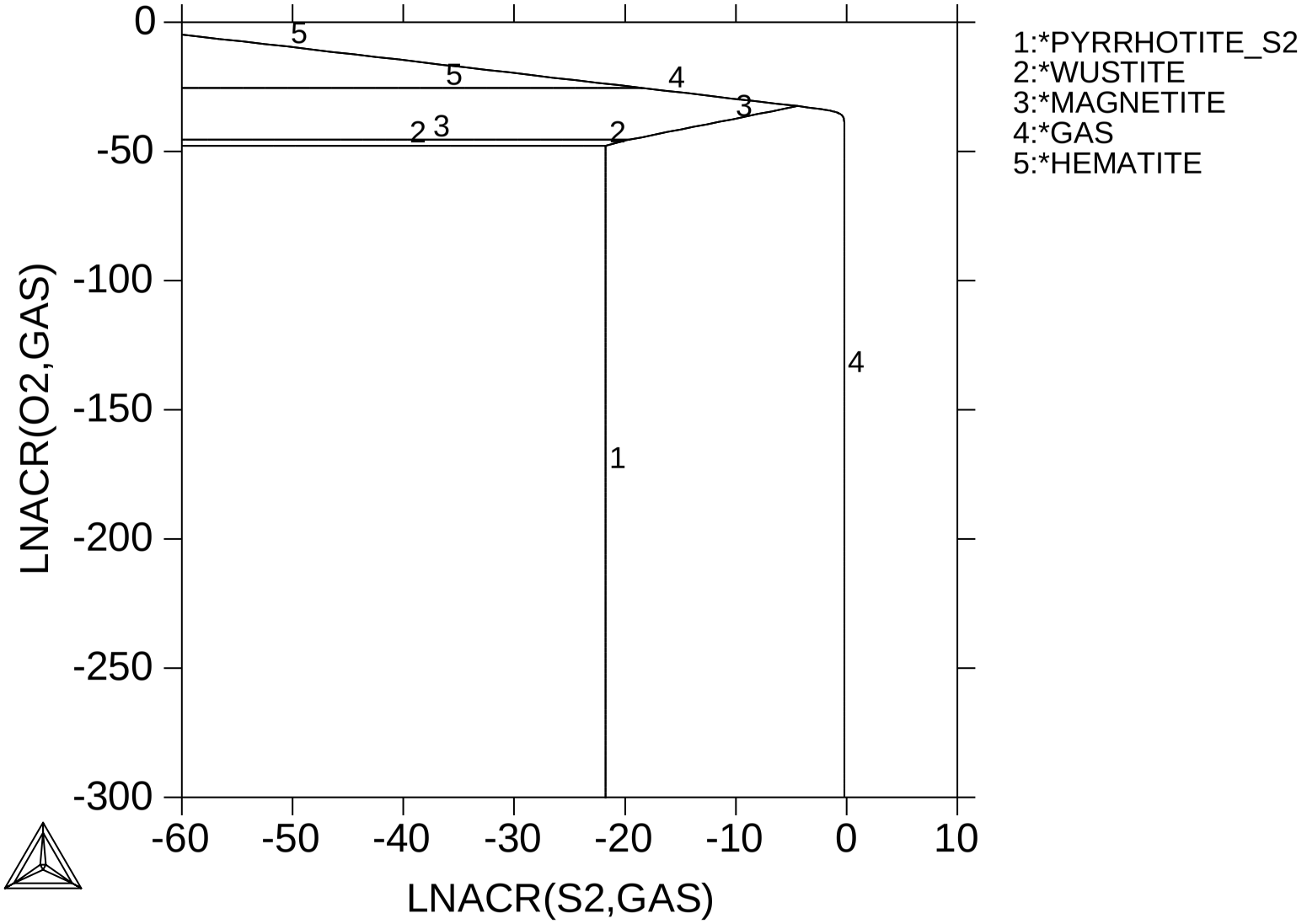
Phase region boundary  22 at:  -1.409E+02 -4.780E+01
    FE
 ** WUSTITE
Calculated.           61  equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: POT.POLY3
CPU time for mapping           8  seconds

 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

Setting automatic diagram axis

POST: s-s x n -80 10
POST: s-s x n -60 10
POST: set-title example 35a
POST: @@ to have all lines solid, use SET-PLOT-OPT and answer Y to ALWAYS SOLID LINES
POST: s-p-o
PLOT HEADER /Y/:  Y
PLOT LOGO /Y/:  Y
PLOT FOOTER /Y/:  Y
WHITE-CONTOURED-PS-CHARS /N/:  N
PLOT REMOTE EXPONENT(S) /Y/:  Y
PLOT SYMBOLS AT NODE POINTS /0/:  0
SYMBOL SIZE /.1/:  0.1
WRITE CONDITIONS? /Y/:  Y
WRITE DATABASE NAME? /Y/:  Y
Always initiate POST on re-entering: /Y/:  Y
Always solid line: /N/:  Y
POST: pl
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
POST: CPU time           8  seconds
```

THERMO-CALC (2009.04.15:03.08) :example 35a
DATABASE:PSUB
P=1E5, N=1, T=1000;



36

Assessment
The use of the PARROT module

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@ This is the setup file for unix systems
SYS: @@
SYS: set_log tcex36a,,,,
SYS: @@ First the elements and phases must be entered in G-E-S module
SYS: GO G
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
 First version released 1-Jan-78, last update 20-Nov-2007

GES: ENTER-ELEMENT A B
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
GES: AMEND-ELEMENT-DATA A BCC 20 0 0 1
GES: AMEND-ELEMENT-DATA B BCC 50 0 0 1
GES: ENTER-PHASE LIQUID L 1 A B; N N
GES: ENTER-PHASE BCC,, 1 A B; N N
GES: ENTER-PHASE FCC,, 1 A B; N N
GES: ENTER-PHASE A2B,, 2 2 1 A; B; N N
 CONSTITUENTS IN SUBLATTICE           1
 CONSTITUENTS IN SUBLATTICE           2
GES: @@ There is a miscibility gap in the bcc, this must be stated here
GES: AMEND_PHASE BCC COMPOSITION_SETS 2 B
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES: @@ We can also set the major constituent of the first composition set
GES: AMEND_PHASE BCC MAJOR 1 A
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: @@ The FCC phase is stable only for element B
GES: AMEND_PHASE FCC MAJOR 1 B
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES: @@ the parameters can be entered in the PARROT module
GES: GO PAR
   ... the command in full is GOTO_MODULE

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: ENTER-PARAMETER G(BCC,A) 500 0; 2000 N
 G(BCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(BCC,B) 500 0; 2000 N
 G(BCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A) 500 14000-10*T; 2000 N
 G(LIQUID,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(LIQUID,B) 500 18000-12*T; 2000 N
 G(LIQUID,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,B) 500 3300-3*T; 2000 N
 G(FCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,A) 500 408; 2000 N
 G(FCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(A2B) 500 V1+V2*T+V3*T*LOG(T); 2000 N
 G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;0) 500 V11+V12*T; 2000 N
 G(LIQUID,A,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;1) 500 V13+V14*T; 2000 N
 G(LIQUID,A,B;1)
PARROT: ENTER-PARAMETER G(BCC,A,B;0) 500 V15+V16*T; 2000 N
 G(BCC,A,B;0)
PARROT: ENTER-PARAMETER G(BCC,A,B;1) 500 V17+V18*T; 2000 N
 G(BCC,A,B;1)
PARROT: ENTER-PARAMETER G(FCC,A,B;0) 500 V19+V20*T; 2000 N
 G(FCC,A,B;0)
PARROT: ENTER-PARAMETER G(FCC,A,B;1) 500 V21+V22*T; 2000 N
```

G(FCC,A,B;1)
PARROT:
PARROT:
PARROT: ***@@ everything is saved on an unformatted work file by the create command***
PARROT: **CREATE tcex36**
... the command in full is CREATE_NEW_STORE_FILE
PARROT:
PARROT: **@?<Hit_return_to_continue>**
PARROT:
PARROT: ***@@ the experimental data file is compiled to the work file.***
PARROT: **COMPILE tcex36 screen Y tcex36.exp**
... the command in full is COMPILE_EXPERIMENTS
A new feature is that POP files may include graphics information using the
GRAPHICS_PLOT command. A file name for generating an ".exp" file must be given.
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is LABEL_DATA
... the command in full is SET_ALTERNATE_CONDITION
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is GRAPHICS_PLOT
... the command in full is LABEL_DATA
... the command in full is SET_ALTERNATE_CONDITION
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is SET_ALTERNATE_CONDITION
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is LABEL_DATA
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is LABEL_DATA
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is SET_ALTERNATE_CONDITION
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is LABEL_DATA
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is LABEL_DATA
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is LABEL_DATA
... the command in full is GRAPHICS_PLOT
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is LABEL_DATA
... the command in full is GRAPHICS_PLOT
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is LABEL_DATA
... the command in full is GRAPHICS_PLOT
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is LABEL_DATA
... the command in full is GRAPHICS_PLOT
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is LABEL_DATA
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
... the command in full is GRAPHICS_PLOT
... the command in full is GRAPHICS_PLOT
... the command in full is LABEL_DATA
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set

```
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
   ... the command in full is GRAPHICS_PLOT
   ... the command in full is LABEL_DATA
   ... the command in full is SET_ALL_START_VALUES
 Automatic start values will be set
PARROT:
PARROT: @@
PARROT: @@ Next file shows how to guess rough start guess of the coefficients
PARROT: @@ and run the actual assessment. The values below are the final result.
PARROT: @@ S-O-V 1 20450,,,,,,
PARROT: @@ S-O-V 2 -30.386,,,,,,,
PARROT: @@ S-O-V 3 0.131,,,,,,
PARROT: @@ S-O-V 11 -21817,,,,,
PARROT: @@ S-O-V 12 15.34,,,,,,,,
PARROT: @@ S-O-V 15 24212,,,,,,
```

PARROT: **_@@ S-O-V 16 -8.328,,,,,,,,_**
PARROT: **_@@ S-O-V 17 3105,,,,,,_**
PARROT: **_@@ S-O-V 19 22030,,,,,,_**
PARROT: **_@@ S-O-V 20 -6.981,,,,,,,,_**
PARROT: **_@@ save the start guess on the work file_**
PARROT: **S-O-V 1 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: **S-O-V 2 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: **S-O-V 11 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: **S-O-V 12 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: **S-O-V 15 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: **S-O-V 16 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: **S-O-V 17 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: **S-O-V 19 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: **S-O-V 20 0**
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT:
PARROT: **save**
   ... the command in full is SAVE_PARROT_WORKSPACES
PARROT:
PARROT: **EXIT**
Are you sure? /NO/: **YES**
 CPU time   0 seconds

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@ Assessment example 36. Version P or later of Thermo-Calc needed
SYS: @@ The macro file tcex36a.TCM must first be used to create the store
SYS: @@ file tcex36.PAR and compile the experiments from tcex36.POP
SYS: @@
SYS: set-log tcex36b,,,
SYS: go par
   ... the command in full is GOTO_MODULE

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: s-s-f tcex36
   ... the command in full is SET_STORE_FILE
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
   ... the command in full is LIST_ALL_VARIABLES
FILE NAME: /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT: @@ Set alt mode (new in version M) to start
PARROT: s-alt
   ... the command in full is SET_ALTERNATE_MODE
On? /Y/:  Y
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read
   ... the command in full is READ_WORKSPACES
Block number /1/:  1
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV *alt*  1.0  1193.0      LIQUID A2B BCC
   2 AINV *alt*  1.0  1341.0      LIQUID A2B
   3 AINV *alt*  1.0  1049.0      LIQUID A2B BCC
   4 AINV *alt*  1.0  1203.0      LIQUID BCC FCC
   5 AINV *alt*  1.0   726.0      A2B BCC BCC#2
   6 AINV *alt*  1.0   726.0      BCC BCC#2
 Failed using alternate for FCC#1                      setting weight to zero
  10 ALF  *alt*  1.0  1594.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  11 ALF  *alt*  1.0  1548.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  12 ALF  *alt*  1.0  1499.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  13 ALF  *alt*  1.0  1438.0      LIQUID FCC
  20 ATIE *alt*  1.0  1413.0      LIQUID FCC
  21 ATIE *alt*  1.0  1337.0      LIQUID FCC
  22 ATIE *alt*  1.0  1213.0      LIQUID FCC
  23 ATIE *alt*  1.0  1100.0      LIQUID BCC
```

```
 100 AA     5   1.    1573.0      LIQUID
 101 AA     4   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     3   1.    1573.0      LIQUID
 104 AA     4   1.    1573.0      LIQUID
 105 AA     6   1.    1573.0      LIQUID
 106 AA     8   1.    1573.0      LIQUID
 107 AA     9   1.    1573.0      LIQUID
 108 AA    11   1.    1573.0      LIQUID
 110 AH     8   1.    1773.0      LIQUID
 111 AH     6   1.    1773.0      LIQUID
 112 AH     5   1.    1773.0      LIQUID
 113 AH     3   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     3   1.    1773.0      LIQUID
 116 AH     5   1.    1773.0      LIQUID
 117 AH     7   1.    1773.0      LIQUID
 118 AH     8   1.    1773.0      LIQUID
 Number of alternate equilibria          14
ED_EXP: @@ Equilibra with label ALF cannot use alt mode
ED_EXP: s-we 0 alf
   ... the command in full is SET_WEIGHT
 Changed weight on            4  equilibria.
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes of weights before leaving editor
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ Optimize zero times as a check
PARROT: opt
   ... the command in full is OPTIMIZE_VARIABLES
Number of iterations /100/:  0
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  C
FILE NAME: /SCREEN/:

          ================================================
          OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57: 7

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
```

```
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   1.22023362E+03
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   3.21114110E+01

 Number of alternate equilibria           10

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)

 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T

 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)

 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: 0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: 0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T

 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: 408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                    1.81
   2 Alternate equilibrium calc                                    0.39
2 HTR=3727                      1.5333E+04  5.00E+02  1.1606E+04   23.21    *
   3 Alternate equilibrium calc                                    1.32
   4 Alternate equilibrium calc                                    1.56
   5 Alternate equilibrium calc                                    4.14
   6 Alternate equilibrium calc                                    3.83
  20 Alternate equilibrium calc                                    0.87
  21 Alternate equilibrium calc                                    0.97
  22 Alternate equilibrium calc                                    1.14
  23 Alternate equilibrium calc                                    1.20
100 ACR(B)=0.94                 0.9382      2.89E-02 -1.8474E-03 -6.3948E-02
101 ACR(B)=0.84                 0.8339      2.89E-02 -6.0866E-03 -0.2107
102 ACR(B)=0.74                 0.7297      2.89E-02 -1.0326E-02 -0.3574
103 ACR(B)=0.64                 0.6254      2.89E-02 -1.4565E-02 -0.5042
104 ACR(B)=0.54                 0.5212      2.89E-02 -1.8804E-02 -0.6509
105 ACR(B)=0.44                 0.4170      2.89E-02 -2.3043E-02 -0.7976
106 ACR(B)=0.34                 0.3127      2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23                 0.2085      2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12                 0.1042      2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964            0.000      5.00E+02   1964.       3.928
111 HMR(LIQUID)=-3500           3.6380E-12  5.00E+02   3500.       7.000    *
112 HMR(LIQUID)=-4588            0.000      5.00E+02   4588.       9.176    *
113 HMR(LIQUID)=-5239            0.000      5.00E+02   5239.       10.48    *
114 HMR(LIQUID)=-5454           3.6380E-12  5.00E+02   5454.       10.91    *
```

```
115 HMR(LIQUID)=-5233           1.8190E-12  5.00E+02   5233.       10.47    *
116 HMR(LIQUID)=-4575            0.000      5.00E+02   4575.       9.150    *
117 HMR(LIQUID)=-3481           1.8190E-12  5.00E+02   3481.       6.962    *
118 HMR(LIQUID)=-1950           1.8190E-12  5.00E+02   1950.       3.900

PARROT: @?<Hit_return_to_continue>
PARROT: @@ Note only one error from alternate calculations. This error represents
PARROT: @@ the difference in chemical potentials of the phases.
PARROT: @@ Experiments with just one phase is calculated as normal.
PARROT: @@ Next command supresses listing of parameters.
PARROT: s-o-l
   ... the command in full is SET_OUTPUT_LEVELS
LIST INCREMENT: /1/:  1
LIST SUM OF SQUARES? /Y/:  Y
LIST SCALED VARIABLES? /Y/:  Y
LIST WEIGHTED RESIDUALS? /N/:  N
LIST ALL PARAMETERS? /Y/:  n
LIST CORRELATION MATRIX? /N/:  N
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  C
FILE NAME: /SCREEN/:

          ================================================
          OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57: 7

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   1.22023362E+03
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   3.21114110E+01

 Number of alternate equilibria           10

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                      1.81
   2 Alternate equilibrium calc                                      0.39
2 HTR=3727                      1.5333E+04  5.00E+02  1.1606E+04   23.21    *
   3 Alternate equilibrium calc                                      1.32
   4 Alternate equilibrium calc                                      1.56
   5 Alternate equilibrium calc                                      4.14
   6 Alternate equilibrium calc                                      3.83
  20 Alternate equilibrium calc                                      0.87
  21 Alternate equilibrium calc                                      0.97
  22 Alternate equilibrium calc                                      1.14
```

```
  23 Alternate equilibrium calc                                        1.20
100 ACR(B)=0.94                  0.9382      2.89E-02 -1.8474E-03 -6.3948E-02
101 ACR(B)=0.84                  0.8339      2.89E-02 -6.0866E-03 -0.2107
102 ACR(B)=0.74                  0.7297      2.89E-02 -1.0326E-02 -0.3574
103 ACR(B)=0.64                  0.6254      2.89E-02 -1.4565E-02 -0.5042
104 ACR(B)=0.54                  0.5212      2.89E-02 -1.8804E-02 -0.6509
105 ACR(B)=0.44                  0.4170      2.89E-02 -2.3043E-02 -0.7976
106 ACR(B)=0.34                  0.3127      2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23                  0.2085      2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12                  0.1042      2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964             0.000      5.00E+02   1964.       3.928
111 HMR(LIQUID)=-3500            3.6380E-12  5.00E+02   3500.       7.000    *
112 HMR(LIQUID)=-4588             0.000      5.00E+02   4588.       9.176    *
113 HMR(LIQUID)=-5239             0.000      5.00E+02   5239.       10.48    *
114 HMR(LIQUID)=-5454            3.6380E-12  5.00E+02   5454.       10.91    *
115 HMR(LIQUID)=-5233            1.8190E-12  5.00E+02   5233.       10.47    *
116 HMR(LIQUID)=-4575             0.000      5.00E+02   4575.       9.150    *
117 HMR(LIQUID)=-3481            1.8190E-12  5.00E+02   3481.       6.962    *
118 HMR(LIQUID)=-1950            1.8190E-12  5.00E+02   1950.       3.900

PARROT: @@ Now optimize
PARROT: opt
   ... the command in full is OPTIMIZE_VARIABLES
Number of iterations /0/:  30
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A

     AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    1.22023362E+03
  1  0.0000E+00   2  0.0000E+00   3  0.0000E+00   4  0.0000E+00   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

     AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    1.22023056E+03
  1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  0.0000E+00   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

                         :
                         :
                         :

     AT THE   29 TH ITERATION WE HAVE THE SUM OF SQUARES    9.32175196E+02
  1  2.2754E+00   2 -4.5239E-03   3 -2.4557E+00   4  3.0908E-03   5  2.5156E+00
  6  1.1674E-02   7  3.4709E-01   8 -7.3322E+00   9  1.0740E-02

     AT THE   30 TH ITERATION WE HAVE THE SUM OF SQUARES    9.32266138E+02
  1  2.2754E+00   2 -4.5260E-03   3 -2.4557E+00   4  3.1696E-03   5  2.5156E+00
  6  1.1696E-02   7  3.4708E-01   8 -7.3322E+00   9  1.0745E-02

 *** ERROR RETURN FROM VA05A BECAUSE THERE HAVE BEEN   30 CALLS OF CALFUN

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   30 iterations
  1  2.2754E+00   2 -4.5239E-03   3 -2.4557E+00   4  3.0908E-03   5  2.5156E+00
  6  1.1674E-02   7  3.4709E-01   8 -7.3322E+00   9  1.0740E-02

  1  2.7586E-01   2  2.7586E-01   3 -2.3479E-02   4 -2.9092E-01   5 -1.4825E-01
  6 -2.4894E-01   7  2.0604E+01   8  1.1427E-01   9  1.1427E-01  10 -2.1551E-01
 11 -1.4793E-01  12  6.1401E-02  13 -4.3625E-02  14 -7.7890E-01  15 -8.0449E-02
 16  4.8856E-01  17  4.8856E-01  18 -7.3181E-01  19  1.4636E+00  20 -7.3181E-01
 21  1.4636E+00  22 -4.1620E-01  23 -1.1022E-02  24 -5.4162E-01  25 -2.8760E-02
 26 -7.6572E-01  27 -7.3156E-02  28 -1.2544E-01  29 -1.0373E-01  30 -4.2178E-03
 31  2.5901E-03  32  6.6371E-02  33  1.4719E-01  34  2.0341E-01  35  1.9322E-01
 36  7.6392E-02  37  1.5206E-01  38  3.2167E-02  39  3.4860E+00  40  6.2142E+00
 41  8.1446E+00  42  9.2993E+00  43  9.6801E+00  44  9.2873E+00  45  8.1186E+00
 46  6.1762E+00  47  3.4580E+00

              THE SUM OF SQUARES IS   9.32175196E+02
PARROT: cont
   ... the command in full is CONTINUE_OPTIMIZATION
Number of iterations /30/:  30
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A
```

```
    Optimization continuing with same Jacobian

      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    6.42380264E+02

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    3.93290410E+02

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    2.09584777E+02

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.80934480E+01

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    9.80053983E-01

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    4 iterations
  1  2.0269E+01   2 -2.9190E-02   3 -2.1813E+01   4  1.5556E-02   5  1.9856E+01
  6 -3.2629E-03   7  3.3757E+00   8 -5.2038E+01   9  5.0440E-02

  1 -1.6296E-03   2 -1.6296E-03   3  1.8276E-04   4  1.5453E-01   5  1.3483E-01
  6 -1.3372E-01   7  5.3419E-03   8 -1.9205E-03   9 -1.9205E-03  10  5.9901E-02
 11 -5.3042E-03  12  1.0919E-01  13 -3.1490E-03  14 -3.7871E-01  15 -1.5089E-02
 16  2.6187E-02  17  2.6187E-02  18 -1.0465E-01  19  6.6481E-02  20 -1.0465E-01
 21  6.6481E-02  22  4.7595E-01  23  4.3175E-03  24  1.7990E-01  25 -3.8161E-04
 26 -3.4080E-01  27 -1.0881E-02  28  7.4579E-02  29 -2.7851E-03  30  2.1225E-03
 31  2.5569E-02  32  1.1253E-01  33  2.1861E-01  34  2.9732E-01  35  3.0190E-01
 36  1.8750E-01  37  2.4842E-01  38  9.3002E-02  39  1.7059E-03  40  1.9922E-02
 41  1.4647E-02  42  7.8823E-03  43  1.6274E-03  44 -4.1177E-03  45 -1.1353E-02
 46 -1.8078E-02  47 -2.6294E-02

               THE SUM OF SQUARES IS   9.80053983E-01
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/: C
FILE NAME: /SCREEN/:

           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57: 7

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02691574E+04    0.00000000E+00    1.00000000E+03    1.60588758E+00
 V2     -2.91902483E+01    0.00000000E+00    1.00000000E+03    1.00991503E-02
 V11    -2.18127453E+04    0.00000000E+00    1.00000000E+03    8.65821610E-01
 V12     1.55559533E+01    0.00000000E+00    1.00000000E+03    2.63408160E-03
 V15     1.98563483E+04    0.00000000E+00    1.00000000E+03    1.43532345E+01
 V16    -3.26290214E+00    0.00000000E+00    1.00000000E+03    1.71198704E-02
 V17     3.37569320E+03    0.00000000E+00    1.00000000E+03    4.53503077E+00
 V19    -5.20384274E+04    0.00000000E+00    1.00000000E+03    3.15139060E+01
 V20     5.04396140E+01    0.00000000E+00    1.00000000E+03    2.47933170E-02

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.22023362E+03 TO   9.80053983E-01
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   2.57908943E-02

 Number of alternate equilibria           10

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
```

```
   1 Alternate equilibrium calc                                    0.15
   2 Alternate equilibrium calc                                    0.19
2 HTR=3727                        3730.      5.00E+02   2.671      5.3419E-03
   3 Alternate equilibrium calc                                    0.06
   4 Alternate equilibrium calc                                    0.39
   5 Alternate equilibrium calc                                    0.13
   6 Alternate equilibrium calc                                    0.12
  20 Alternate equilibrium calc                                    0.48
  21 Alternate equilibrium calc                                    0.18
  22 Alternate equilibrium calc                                    0.34
  23 Alternate equilibrium calc                                    0.07
100 ACR(B)=0.94                  0.9401      2.84E-02  6.0224E-05  2.1225E-03
101 ACR(B)=0.84                  0.8407      2.80E-02  7.1692E-04  2.5569E-02
102 ACR(B)=0.74                  0.7431      2.79E-02  3.1370E-03  0.1125
103 ACR(B)=0.64                  0.6461      2.79E-02  6.0968E-03  0.2186
104 ACR(B)=0.54                  0.5483      2.81E-02  8.3480E-03  0.2973
105 ACR(B)=0.44                  0.4486      2.85E-02  8.5910E-03  0.3019
106 ACR(B)=0.34                  0.3454      2.90E-02  5.4463E-03  0.1875
107 ACR(B)=0.23                  0.2374      2.99E-02  7.4228E-03  0.2484
108 ACR(B)=0.12                  0.1229      3.10E-02  2.8825E-03  9.3002E-02
110 HMR(LIQUID)=-1964            -1963.      5.00E+02  0.8529      1.7059E-03
111 HMR(LIQUID)=-3500            -3490.      5.00E+02   9.961      1.9922E-02
112 HMR(LIQUID)=-4588            -4581.      5.00E+02   7.323      1.4647E-02
113 HMR(LIQUID)=-5239            -5235.      5.00E+02   3.941      7.8823E-03
114 HMR(LIQUID)=-5454            -5453.      5.00E+02  0.8137      1.6274E-03
115 HMR(LIQUID)=-5233            -5235.      5.00E+02  -2.059     -4.1177E-03
116 HMR(LIQUID)=-4575            -4581.      5.00E+02  -5.677     -1.1353E-02
117 HMR(LIQUID)=-3481            -3490.      5.00E+02  -9.039     -1.8078E-02
118 HMR(LIQUID)=-1950            -1963.      5.00E+02  -13.15     -2.6294E-02

PARROT:
PARROT:
PARROT: @?<Hit_return_to_continue>
PARROT: @@ The liquid data fitted reasonable, fix its parameters to simplify
PARROT: l-p-d liq
   ... the command in full is LIST_PHASE_DATA

 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T
PARROT: s-f-v 11-14
   ... the command in full is SET_FIX_VARIABLE
PARROT: @@ Rescale the start values of the parameters to current values
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: l-a-v
   ... the command in full is LIST_ALL_VARIABLES
FILE NAME: /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02691574E+04    2.02691574E+04    2.02691574E+04    0.00000000E+00
 V2     -2.91902483E+01   -2.91902483E+01   -2.91902483E+01    0.00000000E+00
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     1.98563483E+04    1.98563483E+04    1.98563483E+04    0.00000000E+00
 V16    -3.26290214E+00   -3.26290214E+00   -3.26290214E+00    0.00000000E+00
 V17     3.37569320E+03    3.37569320E+03    3.37569320E+03    0.00000000E+00
 V19    -5.20384274E+04   -5.20384274E+04   -5.20384274E+04    0.00000000E+00
 V20     5.04396140E+01    5.04396140E+01    5.04396140E+01    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT: @?<Hit_return_to_continue>
PARROT: mac tcex36cpd
PARROT: @@ The following commands are in the file tcex36cpd.TCM
```

```
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be runned in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          412  grid points in           0  s
 Found the set of lowest grid points in           0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
```

```
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   8.907E-02  3.100E+02
     BCC#1
  ** FCC
 *** Buffer saved on file: tcex36.POLY3
 Calculated..            2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   8.956E-02  3.000E+02
     BCC#1
  ** FCC
 Calculated.           29  equilibria

 Phase region boundary   3 at:   1.213E-01  1.253E+03
  ** LIQUID
     BCC#1
  ** FCC

 Phase region boundary   4 at:   2.038E-01  1.253E+03
  ** LIQUID
     BCC#1
 Calculated           23  equilibria

       :
       :
       :

 Phase region boundary  35 at:   6.122E-01  1.246E+03
     LIQUID
  ** A2B
 Calculated.           13  equilibria
 Terminating at known equilibrium

 Phase region boundary  36 at:   6.122E-01  1.246E+03
     LIQUID
  ** A2B
 Calculated.            4  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   9.944E-01  1.601E+03
     LIQUID
  ** FCC
 Calculated.           33  equilibria
 Terminating at known equilibrium

 Phase region boundary  38 at:   9.944E-01  1.601E+03
     LIQUID
  ** FCC
 Calculated           12  equilibria
 *** BUFFER SAVED ON FILE: tcex36.POLY3
 CPU time for mapping           2  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis
```

```
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
PLOTFILE : /SCREEN/:
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-inter
POST:
POST: @@ End of commands from tcex36cpd.TCM and back in tcex36b.TCM now
POST:
POST: @?<Hit_return_to_continue>
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt
   ... the command in full is OPTIMIZE_VARIABLES
Number of iterations /30/:  30
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use     824 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A

     AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    9.80053983E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    9.80046615E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

                         :
                         :
                         :

     AT THE   17 TH ITERATION WE HAVE THE SUM OF SQUARES    4.93884034E-01
  1  9.9983E-01   2  9.9618E-01   3  1.1210E+00   4  1.8221E+00   5  9.5929E-01
  6  1.9649E-01   7  3.5984E-01

     AT THE   18 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83962160E-01
  1  1.0003E+00   2  9.9394E-01   3  1.2080E+00   4  2.4585E+00   5  9.2882E-01
  6 -4.0863E-01   7 -1.2364E-01

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   18 iterations
  1  1.0003E+00   2  9.9394E-01   3  1.2080E+00   4  2.4585E+00   5  9.2882E-01
  6 -4.0863E-01   7 -1.2364E-01

  1  5.6826E-03   2  5.6826E-03   3 -5.2703E-04   4 -1.0121E-03   5  1.2997E-01
  6 -1.3615E-01   7  9.2250E-04   8  5.4224E-03   9  5.4224E-03  10  5.3337E-04
 11 -6.9114E-03  12  2.1376E-03  13 -5.6500E-03  14  2.0876E-03  15 -5.3921E-03
 16  9.5281E-03  17  9.5281E-03  18  2.1204E-04  19 -3.0972E-03  20  2.1204E-04
 21 -3.0972E-03  22 -2.1113E-03  23 -3.4455E-04  24  3.5839E-03  25 -3.0619E-03
 26 -3.2846E-03  27 -2.5884E-03  28 -6.7138E-04  29 -4.9773E-03  30  2.1225E-03
 31  2.5569E-02  32  1.1253E-01  33  2.1861E-01  34  2.9732E-01  35  3.0190E-01
 36  1.8750E-01  37  2.4842E-01  38  9.3002E-02  39  1.7059E-03  40  1.9922E-02
 41  1.4647E-02  42  7.8823E-03  43  1.6274E-03  44 -4.1177E-03  45 -1.1353E-02
 46 -1.8078E-02  47 -2.6294E-02

              THE SUM OF SQUARES IS   3.83962160E-01
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt
   ... the command in full is OPTIMIZE_VARIABLES
Number of iterations /30/:  30
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use     824 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A
```

```
     AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83962160E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    3.83964036E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    3.83962249E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    3.83962784E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83962209E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83962166E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83962255E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83962174E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0001E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    7 iterations
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

  1  5.6826E-03   2  5.6826E-03   3 -5.2703E-04   4 -1.0121E-03   5  1.2997E-01
  6 -1.3615E-01   7  9.2250E-04   8  5.4224E-03   9  5.4224E-03  10  5.3337E-04
 11 -6.9114E-03  12  2.1376E-03  13 -5.6500E-03  14  2.0876E-03  15 -5.3921E-03
 16  9.5281E-03  17  9.5281E-03  18  2.1204E-04  19 -3.0972E-03  20  2.1204E-04
 21 -3.0972E-03  22 -2.1113E-03  23 -3.4455E-04  24  3.5839E-03  25 -3.0619E-03
 26 -3.2846E-03  27 -2.5884E-03  28 -6.7138E-04  29 -4.9773E-03  30  2.1225E-03
 31  2.5569E-02  32  1.1253E-01  33  2.1861E-01  34  2.9732E-01  35  3.0190E-01
 36  1.8750E-01  37  2.4842E-01  38  9.3002E-02  39  1.7059E-03  40  1.9922E-02
 41  1.4647E-02  42  7.8823E-03  43  1.6274E-03  44 -4.1177E-03  45 -1.1353E-02
 46 -1.8078E-02  47 -2.6294E-02

             THE SUM OF SQUARES IS   3.83962160E-01
PARROT: @@ No change in the parameters, check the diagram again
PARROT: mac tcex36cpd
PARROT: @@ The following commands are in the file tcex36cpd.TCM
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be runned in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
```

```
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          412  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC#1
  ** BCC#2
```

```
 Calculated..            2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
    BCC#1
  ** BCC#2
 Calculated.           14  equilibria

 Phase region boundary   3 at:   6.802E-01  7.347E+02
  ** A2B
    BCC#1
  ** BCC#2

 Phase region boundary   4 at:   3.640E-01  7.347E+02
  ** A2B
    BCC#1
 Calculated.           14  equilibria

       :
       :
       :

 Phase region boundary  39 at:   6.122E-01  1.219E+03
    LIQUID
  ** A2B
 Calculated.           12  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.219E+03
    LIQUID
  ** A2B
 Calculated.            7  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
    LIQUID
  ** FCC
 Calculated.           20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
    LIQUID
  ** FCC
 Calculated          13  equilibria
 *** BUFFER SAVED ON FILE: tcex36.POLY3
 CPU time for mapping          2  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
PLOTFILE : /SCREEN/:
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-inter
POST:
POST: @@ End of commands from tcex36cpd.TCM and back in tcex36b.TCM now
POST:
POST: @?<Hit_return_to_continue>
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Turn off alternate mode and try to calculate all equilibria
PARROT: s-alt
   ... the command in full is SET_ALTERNATE_MODE
```

```
 Alternate calculation is on
Off? /Y/: Y
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read
   ... the command in full is READ_WORKSPACES
Block number /1/: 1
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   3   1.    1187.5      LIQUID A2B BCC
   2 AINV   2   1.    1316.7      LIQUID A2B
   3 AINV   3   1.    1047.0      LIQUID A2B BCC
   4 AINV   3   1.    1204.7      LIQUID BCC FCC
   5 AINV   4   1.     734.7      A2B BCC BCC#2
   6 AINV   3   1.     726.0      BCC BCC#2
  10 ALF  < unused >  1594.0      LIQUID FCC
  11 ALF  < unused >  1548.0      LIQUID FCC
  12 ALF  < unused >  1499.0      LIQUID FCC
  13 ALF  < unused >  1438.0      LIQUID FCC
  20 ATIE   3   1.    1413.0      LIQUID FCC
  21 ATIE   3   1.    1337.0      LIQUID FCC
  22 ATIE   3   1.    1213.0      LIQUID FCC
  23 ATIE   3   1.    1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     2   1.    1773.0      LIQUID
 116 AH     2   1.    1773.0      LIQUID
 117 AH     2   1.    1773.0      LIQUID
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
ED_EXP: @@ any liquid parameters and restore those with label ALF
ED_EXP: s-we 0 100-118
   ... the command in full is SET_WEIGHT
ED_EXP: s-we 1 alf
   ... the command in full is SET_WEIGHT
 Changed weight on           4  equilibria.
ED_EXP: s-e 1
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number           1 , label AINV
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1187.5      LIQUID A2B BCC
   2 AINV   2   1.    1316.7      LIQUID A2B
   3 AINV   2   1.    1047.0      LIQUID A2B BCC
   4 AINV   2   1.    1204.7      LIQUID BCC FCC
   5 AINV   2   1.     734.7      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    6   1.    1594.0      LIQUID FCC
  11 ALF    6   1.    1548.0      LIQUID FCC
  12 ALF    7   1.    1499.0      LIQUID FCC
  13 ALF    7   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA   < unused >  1573.0      LIQUID
 101 AA   < unused >  1573.0      LIQUID
 102 AA   < unused >  1573.0      LIQUID
 103 AA   < unused >  1573.0      LIQUID
 104 AA   < unused >  1573.0      LIQUID
```

```
 105 AA   < unused >  1573.0      LIQUID
 106 AA   < unused >  1573.0      LIQUID
 107 AA   < unused >  1573.0      LIQUID
 108 AA   < unused >  1573.0      LIQUID
 110 AH   < unused >  1773.0      LIQUID
 111 AH   < unused >  1773.0      LIQUID
 112 AH   < unused >  1773.0      LIQUID
 113 AH   < unused >  1773.0      LIQUID
 114 AH   < unused >  1773.0      LIQUID
 115 AH   < unused >  1773.0      LIQUID
 116 AH   < unused >  1773.0      LIQUID
 117 AH   < unused >  1773.0      LIQUID
 118 AH   < unused >  1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  c
FILE NAME: /SCREEN/:

          ================================================
          OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57:12

 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02757864E+04    2.02757864E+04    2.02757864E+04    7.39333291E-02
 V2     -2.90134108E+01   -2.90134108E+01   -2.90134108E+01    3.44753278E-01
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     2.39869526E+04    2.39869526E+04    2.39869526E+04    6.19220658E-01
 V16    -8.02179229E+00   -8.02179229E+00   -8.02179229E+00    2.18789496E+00
 V17     3.13540515E+03    3.13540515E+03    3.13540515E+03    1.44882548E+00
 V19     2.12643614E+04    2.12643614E+04    2.12643614E+04    4.78622176E+00
 V20    -6.23643996E+00   -6.23643996E+00   -6.23643996E+00    1.26468944E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   3.83962160E-01 TO   7.41796469E+00
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   3.37180213E-01

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1187.       10.      -5.532     -0.5532
1 W(LIQUID,B)=0.408              0.4157      2.00E-02  7.7215E-03  0.3861
1 W(BCC#1,B)=0.13                0.1332      2.00E-02  3.2119E-03  0.1606
2 T=1341                          1317.       10.      -24.32      -2.432
2 HTR=3727                        3727.      5.00E+02  0.4611      9.2228E-04
```

```
3 T=1049                          1047.       10.      -1.990     -0.1990
3 W(LIQUID,A)=0.27               0.2739      2.00E-02  3.9062E-03  0.1953
3 W(BCC#1,A)=9.3E-2              9.4971E-02  2.00E-02  1.9713E-03  9.8563E-02
4 T=1203                          1205.       10.       1.671      0.1671
4 W(LIQUID,A)=0.19               0.1919      2.00E-02  1.8666E-03  9.3329E-02
4 W(BCC#1,A)=6.9E-2              6.9780E-02  2.00E-02  7.8012E-04  3.9006E-02
4 W(FCC,A)=6E-2                  6.0794E-02  2.00E-02  7.9444E-04  3.9722E-02
5 T=726                           734.7       10.       8.703      0.8703
5 X(BCC#1,B)=3.7E-2              3.9289E-02  2.00E-02  2.2886E-03  0.1144
5 X(BCC#2,A)=0.114               0.1200      2.00E-02  6.0001E-03  0.3000
6 X(BCC#1,B)=3.7E-2              3.6833E-02  2.00E-02 -1.6665E-04 -8.3327E-03
6 X(BCC#2,A)=0.114               0.1140      2.00E-02 -1.6829E-05 -8.4145E-04
10 W(LIQUID,A)=2E-2              1.9506E-02  2.00E-02 -4.9427E-04 -2.4713E-02
11 W(LIQUID,A)=4.2E-2            4.1827E-02  2.00E-02 -1.7330E-04 -8.6650E-03
12 W(LIQUID,A)=6.5E-2            6.5040E-02  2.00E-02  4.0126E-05  2.0063E-03
13 W(LIQUID,A)=9.3E-2            9.3114E-02  2.00E-02  1.1415E-04  5.7076E-03
20 W(LIQUID,A)=0.104             0.1043      2.00E-02  3.4979E-04  1.7489E-02
20 W(FCC,A)=3.8E-2               3.8244E-02  2.00E-02  2.4396E-04  1.2198E-02
21 W(LIQUID,A)=0.136             0.1375      2.00E-02  1.5283E-03  7.6417E-02
21 W(FCC,A)=4.7E-2               4.7395E-02  2.00E-02  3.9495E-04  1.9747E-02
22 W(LIQUID,A)=0.187             0.1886      2.00E-02  1.5692E-03  7.8458E-02
22 W(FCC,A)=5.9E-2               6.0019E-02  2.00E-02  1.0193E-03  5.0967E-02
23 W(LIQUID,A)=0.245             0.2474      2.00E-02  2.3699E-03  0.1185
23 W(BCC#1,A)=8.5E-2             8.6337E-02  2.00E-02  1.3367E-03  6.6833E-02

PARROT: @?<Hit_return_to_continue>
PARROT: @@ When we optimize zero times we sometimes find an error for equilibrium 4
PARROT: @@ It can be on the wrong side, at high A instead of high B. Try to correct
PARROT: @@ that in the edit module.
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read
   ... the command in full is READ_WORKSPACES
Block number /1/:  1
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number            4 , label AINV
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.671473/:  1200
Automatic start values for phase constituents? /N/:  N
 Phase LIQUID
Major constituent(s):  b
 Phase BCC
Major constituent(s) /b/:  b
 Phase FCC
Major constituent(s) /b/:  b
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=1   FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1204.67 K (   931.52 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.29910E+02
 Total Gibbs energy -9.73780E+03,  Enthalpy  1.97627E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.6967E-01  1.0310E-01 4.0116E-01 -9.1489E+03 SER
 B                       2.3303E+00  8.9690E-01 8.5667E-01 -1.5496E+03 SER

 FCC                          Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5821E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.39206E-01  A  6.07944E-02
```

```
 BCC#1                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5262E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.30220E-01  A  6.97801E-02

 LIQUID                     Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.8826E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.08133E-01  A  1.91867E-01

 EXPERIMENT T=1203:DT  $1204.67:10  NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX  $0.191867:2E-2  NO=2
 EXPERIMENT W(BCC#1,A)=6.9E-2:DX  $6.97801E-2:2E-2  NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX  $6.07944E-2:2E-2  NO=4
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ The error is still there, calculate the phase diagram!!!
PARROT: mac tcex36cpd
PARROT: @@ The following commands are in the file tcex36cpd.TCM
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be runned in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          412  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
```

```
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC#1
  ** BCC#2
 Calculated..             2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC#1
  ** BCC#2
 Calculated.            14  equilibria

 Phase region boundary   3 at:   6.802E-01  7.347E+02
  ** A2B
     BCC#1
  ** BCC#2

 Phase region boundary   4 at:   3.640E-01  7.347E+02
  ** A2B
     BCC#1
 Calculated.            14  equilibria

       :
       :
       :

 Phase region boundary  39 at:   6.122E-01  1.219E+03
     LIQUID
  ** A2B
 Calculated.            12  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.219E+03
     LIQUID
  ** A2B
 Calculated.             7  equilibria
 Terminating at known equilibrium
```

```
 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.           20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated           13  equilibria
 *** BUFFER SAVED ON FILE: tcex36.POLY3
 CPU time for mapping           2  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
PLOTFILE : /SCREEN/:
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-inter
POST:
POST: @@ End of commands from tcex36cpd.TCM and back in tcex36b.TCM now
POST:
POST: @?<Hit_return_to_continue>
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read
   ... the command in full is READ_WORKSPACES
Block number /1/:  1
ED_EXP: s-we 0 4
   ... the command in full is SET_WEIGHT
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use      25 experiments, maximum is        2000
 Use     494 real workspace, maximum is    50000
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  C
FILE NAME: /SCREEN/:

           ================================================
           OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57:14

 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
```

```
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02757864E+04    2.02757864E+04    2.02757864E+04    7.39333291E-02
 V2     -2.90134108E+01   -2.90134108E+01   -2.90134108E+01    3.44753278E-01
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     2.39869526E+04    2.39869526E+04    2.39869526E+04    6.19220658E-01
 V16    -8.02179229E+00   -8.02179229E+00   -8.02179229E+00    2.18789496E+00
 V17     3.13540515E+03    3.13540515E+03    3.13540515E+03    1.44882548E+00
 V19     2.12643614E+04    2.12643614E+04    2.12643614E+04    4.78622176E+00
 V20    -6.23643996E+00   -6.23643996E+00   -6.23643996E+00    1.26468944E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   3.83962160E-01 TO   7.37821696E+00
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   4.09900942E-01

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1187.       10.      -5.532     -0.5532
1 W(LIQUID,B)=0.408              0.4157      2.00E-02  7.7215E-03  0.3861
1 W(BCC#1,B)=0.13                0.1332      2.00E-02  3.2119E-03  0.1606
2 T=1341                          1317.       10.      -24.32      -2.432
2 HTR=3727                        3727.      5.00E+02  0.4611      9.2228E-04
3 T=1049                          1047.       10.      -1.990     -0.1990
3 W(LIQUID,A)=0.27               0.2739      2.00E-02  3.9062E-03  0.1953
3 W(BCC#1,A)=9.3E-2              9.4971E-02  2.00E-02  1.9713E-03  9.8563E-02
5 T=726                           734.7       10.       8.703      0.8703
5 X(BCC#1,B)=3.7E-2              3.9289E-02  2.00E-02  2.2886E-03  0.1144
5 X(BCC#2,A)=0.114               0.1200      2.00E-02  6.0001E-03  0.3000
6 X(BCC#1,B)=3.7E-2              3.6833E-02  2.00E-02 -1.6665E-04 -8.3327E-03
6 X(BCC#2,A)=0.114               0.1140      2.00E-02 -1.6829E-05 -8.4145E-04
10 W(LIQUID,A)=2E-2              1.9506E-02  2.00E-02 -4.9427E-04 -2.4713E-02
11 W(LIQUID,A)=4.2E-2            4.1827E-02  2.00E-02 -1.7330E-04 -8.6650E-03
12 W(LIQUID,A)=6.5E-2            6.5040E-02  2.00E-02  4.0126E-05  2.0063E-03
13 W(LIQUID,A)=9.3E-2            9.3114E-02  2.00E-02  1.1415E-04  5.7076E-03
20 W(LIQUID,A)=0.104             0.1043      2.00E-02  3.4979E-04  1.7489E-02
20 W(FCC,A)=3.8E-2               3.8244E-02  2.00E-02  2.4396E-04  1.2198E-02
21 W(LIQUID,A)=0.136             0.1375      2.00E-02  1.5283E-03  7.6417E-02
21 W(FCC,A)=4.7E-2               4.7395E-02  2.00E-02  3.9495E-04  1.9747E-02
22 W(LIQUID,A)=0.187             0.1886      2.00E-02  1.5692E-03  7.8458E-02
22 W(FCC,A)=5.9E-2               6.0019E-02  2.00E-02  1.0193E-03  5.0967E-02
23 W(LIQUID,A)=0.245             0.2474      2.00E-02  2.3699E-03  0.1185
23 W(BCC#1,A)=8.5E-2             8.6337E-02  2.00E-02  1.3367E-03  6.6833E-02

PARROT: @?<Hit_return_to_continue>
PARROT: opt
   ... the command in full is OPTIMIZE_VARIABLES
Number of iterations /0/:  30
 Use      25 experiments, maximum is        2000
 Use     494 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A

      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    7.37821696E+00
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    7.53023516E+00
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

                        :
                        :
                        :
```

```
     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    2.16951567E-01
  1  9.9691E-01   2  1.0034E+00   3  9.9639E-01   4  9.8058E-01   5  9.8548E-01
  6  1.0080E+00   7  1.0160E+00

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.51361771E-01
  1  9.9564E-01   2  1.0029E+00   3  9.8912E-01   4  9.5293E-01   5  9.6407E-01
  6  1.0089E+00   7  1.0123E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   12 iterations
  1  9.9564E-01   2  1.0029E+00   3  9.8912E-01   4  9.5293E-01   5  9.6407E-01
  6  1.0089E+00   7  1.0123E+00

  1  7.0456E-02   2 -3.9714E-02   3 -7.7916E-02   4 -7.3555E-02   5  5.9816E-02
  6  2.5625E-01   7 -1.8710E-02   8 -9.5446E-02   9  1.6592E-01  10  5.4873E-02
 11 -3.7948E-02  12  3.1686E-02  13 -9.3444E-02  14 -2.8662E-02  15 -1.6941E-02
 16 -1.0568E-02  17 -1.1806E-02  18 -1.9275E-03  19 -9.4027E-03  20  5.1591E-02
 21 -1.0494E-02  22  4.5737E-02  23  2.4188E-03  24  1.2336E-02  25 -8.0307E-02

             THE SUM OF SQUARES IS   1.51361771E-01
PARROT: cont
   ... the command in full is CONTINUE_OPTIMIZATION

 It is safe to CONTINUE only after TOO MANY ITERATIONS
 and no change in variables and experiments ...
 Now anything can happen ...

Are you sure? /N/:  30
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  c
FILE NAME: /SCREEN/:

          ==================================================
          OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57:14

 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  13

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.01874456E+04    2.02757864E+04    2.02757864E+04    2.69317786E-02
 V2     -2.90969461E+01   -2.90134108E+01   -2.90134108E+01    1.50773104E-02
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     2.37258699E+04    2.39869526E+04    2.39869526E+04    9.90009473E-02
 V16    -7.64417506E+00   -8.02179229E+00   -8.02179229E+00    3.01534370E-01
 V17     3.02274877E+03    3.13540515E+03    3.13540515E+03    2.49736605E-01
 V19     2.14534176E+04    2.12643614E+04    2.12643614E+04    6.60456104E-01
 V20    -6.31333528E+00   -6.23643996E+00   -6.23643996E+00    1.71543931E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   7.37821696E+00 TO   1.51361771E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.40898729E-03

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
```

```
1 T=1193                          1194.       10.      0.7046      7.0456E-02
1 W(LIQUID,B)=0.408              0.4072      2.00E-02 -7.9428E-04 -3.9714E-02
1 W(BCC#1,B)=0.13                0.1284      2.00E-02 -1.5583E-03 -7.7916E-02
2 T=1341                          1340.       10.     -0.7356     -7.3555E-02
2 HTR=3727                        3757.      5.00E+02   29.91      5.9816E-02
3 T=1049                          1052.       10.       2.562      0.2562
3 W(LIQUID,A)=0.27               0.2696      2.00E-02 -3.7421E-04 -1.8710E-02
3 W(BCC#1,A)=9.3E-2              9.1091E-02  2.00E-02 -1.9089E-03 -9.5446E-02
5 T=726                           727.7       10.       1.659      0.1659
5 X(BCC#1,B)=3.7E-2              3.8097E-02  2.00E-02  1.0975E-03  5.4873E-02
5 X(BCC#2,A)=0.114               0.1132      2.00E-02 -7.5895E-04 -3.7948E-02
6 X(BCC#1,B)=3.7E-2              3.7634E-02  2.00E-02  6.3372E-04  3.1686E-02
6 X(BCC#2,A)=0.114               0.1121      2.00E-02 -1.8689E-03 -9.3444E-02
10 W(LIQUID,A)=2E-2              1.9427E-02  2.00E-02 -5.7324E-04 -2.8662E-02
11 W(LIQUID,A)=4.2E-2            4.1661E-02  2.00E-02 -3.3882E-04 -1.6941E-02
12 W(LIQUID,A)=6.5E-2            6.4789E-02  2.00E-02 -2.1136E-04 -1.0568E-02
13 W(LIQUID,A)=9.3E-2            9.2764E-02  2.00E-02 -2.3612E-04 -1.1806E-02
20 W(LIQUID,A)=0.104             0.1040      2.00E-02 -3.8550E-05 -1.9275E-03
20 W(FCC,A)=3.8E-2                3.7812E-02  2.00E-02 -1.8805E-04 -9.4027E-03
21 W(LIQUID,A)=0.136              0.1370      2.00E-02  1.0318E-03  5.1591E-02
21 W(FCC,A)=4.7E-2                4.6790E-02  2.00E-02 -2.0988E-04 -1.0494E-02
22 W(LIQUID,A)=0.187              0.1879      2.00E-02  9.1474E-04  4.5737E-02
22 W(FCC,A)=5.9E-2                5.9048E-02  2.00E-02  4.8376E-05  2.4188E-03
23 W(LIQUID,A)=0.245              0.2452      2.00E-02  2.4672E-04  1.2336E-02
23 W(BCC#1,A)=8.5E-2              8.3394E-02  2.00E-02 -1.6061E-03 -8.0307E-02

PARROT: @?<Hit_return_to_continue>
PARROT: @@ Optimization converged, try to add equilibrium 4 again
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read
   ... the command in full is READ_WORKSPACES
Block number /1/:  1
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number            4 , label AINV
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.671473/:  1200
Automatic start values for phase constituents? /N/:  N
 Phase LIQUID
Major constituent(s) /b/:  b
 Phase BCC
Major constituent(s) /b/:  b
 Phase FCC
Major constituent(s) /b/:  b
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=1   FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1194.81 K (   921.66 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.29837E+02
 Total Gibbs energy -9.46750E+03,  Enthalpy  1.96784E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.7208E-01  1.0353E-01 4.0897E-01 -8.8824E+03 SER
 B                       2.3279E+00  8.9647E-01 8.5964E-01 -1.5025E+03 SER

 FCC                          Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5830E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.39335E-01  A  6.06654E-02
```

```
 BCC#1                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5327E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.31263E-01  A  6.87372E-02

 LIQUID                     Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.8681E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.04924E-01  A  1.95076E-01

 SET_WEIGHT 0,,,
 EXPERIMENT T=1203:DT
 EXPERIMENT W(LIQUID,A)=0.19:DX
 EXPERIMENT W(BCC#1,A)=6.9E-2:DX
 EXPERIMENT W(FCC,A)=6E-2:DX
ED_EXP: ba
   ... the command in full is BACK
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
PARROT: @@ The following commands are in the file tcex36cpd.TCM
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be runned in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          412  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
```

```
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC#1
  ** BCC#2
 Calculated..             2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC#1
  ** BCC#2
 Calculated.            14  equilibria

 Phase region boundary   3 at:   6.826E-01  7.277E+02
  ** A2B
     BCC#1
  ** BCC#2

 Phase region boundary   4 at:   3.631E-01  7.277E+02
  ** A2B
     BCC#1
 Calculated.            15  equilibria

       :
       :
       :

 Phase region boundary  39 at:   6.122E-01  1.242E+03
     LIQUID
  ** A2B
 Calculated.            13  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.242E+03
     LIQUID
  ** A2B
 Calculated.             8  equilibria
 Terminating at known equilibrium
```

```
 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.           20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated           13  equilibria
 *** BUFFER SAVED ON FILE: tcex36.POLY3
 CPU time for mapping           2  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
PLOTFILE : /SCREEN/:
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-inter
POST:
POST: @@ End of commands from tcex36cpd.TCM and back in tcex36b.TCM now
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Sometimes a very strange shape of the fcc phase here and no
POST: @@ equilibrium between liq, fcc and bcc at high B content.
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  C
FILE NAME: /SCREEN/:

          ================================================
          OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57:16

 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  13

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.01874456E+04    2.02757864E+04    2.02757864E+04    2.69317786E-02
 V2     -2.90969461E+01   -2.90134108E+01   -2.90134108E+01    1.50773104E-02
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     2.37258699E+04    2.39869526E+04    2.39869526E+04    9.90009473E-02
 V16    -7.64417506E+00   -8.02179229E+00   -8.02179229E+00    3.01534370E-01
 V17     3.02274877E+03    3.13540515E+03    3.13540515E+03    2.49736605E-01
 V19     2.14534176E+04    2.12643614E+04    2.12643614E+04    6.60456104E-01
 V20    -6.31333528E+00   -6.23643996E+00   -6.23643996E+00    1.71543931E+00
```

```
 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   7.37821696E+00 TO   1.51361771E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.40898729E-03

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.       10.      0.7046      7.0456E-02
1 W(LIQUID,B)=0.408              0.4072      2.00E-02 -7.9428E-04 -3.9714E-02
1 W(BCC#1,B)=0.13                0.1284      2.00E-02 -1.5583E-03 -7.7916E-02
2 T=1341                          1340.       10.     -0.7356     -7.3555E-02
2 HTR=3727                        3757.      5.00E+02   29.91      5.9816E-02
3 T=1049                          1052.       10.       2.562      0.2562
3 W(LIQUID,A)=0.27               0.2696      2.00E-02 -3.7421E-04 -1.8710E-02
3 W(BCC#1,A)=9.3E-2              9.1091E-02  2.00E-02 -1.9089E-03 -9.5446E-02
5 T=726                           727.7       10.       1.659      0.1659
5 X(BCC#1,B)=3.7E-2              3.8097E-02  2.00E-02  1.0975E-03  5.4873E-02
5 X(BCC#2,A)=0.114               0.1132      2.00E-02 -7.5895E-04 -3.7948E-02
6 X(BCC#1,B)=3.7E-2              3.7634E-02  2.00E-02  6.3372E-04  3.1686E-02
6 X(BCC#2,A)=0.114               0.1121      2.00E-02 -1.8689E-03 -9.3444E-02
10 W(LIQUID,A)=2E-2              1.9427E-02  2.00E-02 -5.7324E-04 -2.8662E-02
11 W(LIQUID,A)=4.2E-2            4.1661E-02  2.00E-02 -3.3882E-04 -1.6941E-02
12 W(LIQUID,A)=6.5E-2            6.4789E-02  2.00E-02 -2.1136E-04 -1.0568E-02
13 W(LIQUID,A)=9.3E-2            9.2764E-02  2.00E-02 -2.3612E-04 -1.1806E-02
20 W(LIQUID,A)=0.104             0.1040      2.00E-02 -3.8550E-05 -1.9275E-03
20 W(FCC,A)=3.8E-2                3.7812E-02  2.00E-02 -1.8805E-04 -9.4027E-03
21 W(LIQUID,A)=0.136              0.1370      2.00E-02  1.0318E-03  5.1591E-02
21 W(FCC,A)=4.7E-2                4.6790E-02  2.00E-02 -2.0988E-04 -1.0494E-02
22 W(LIQUID,A)=0.187              0.1879      2.00E-02  9.1474E-04  4.5737E-02
22 W(FCC,A)=5.9E-2                5.9048E-02  2.00E-02  4.8376E-05  2.4188E-03
23 W(LIQUID,A)=0.245              0.2452      2.00E-02  2.4672E-04  1.2336E-02
23 W(BCC#1,A)=8.5E-2              8.3394E-02  2.00E-02 -1.6061E-03 -8.0307E-02

PARROT:
PARROT: @@ Note that all other experiments are well fitted!
PARROT: @@ Try to improve by optimizing a little more !!!
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt
   ... the command in full is OPTIMIZE_VARIABLES
Number of iterations /30/:  30
 Use      25 experiments, maximum is        2000
 Use     494 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A

      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    1.51361771E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    1.52527143E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

                          :
                          :
                          :

      AT THE   23 TH ITERATION WE HAVE THE SUM OF SQUARES    1.44753968E-01
  1  9.9981E-01   2  9.9992E-01   3  9.9844E-01   4  9.9265E-01   5  9.9546E-01
  6  1.0188E+00   7  1.0468E+00

      AT THE   24 TH ITERATION WE HAVE THE SUM OF SQUARES    1.44421619E-01
  1  9.9973E-01   2  9.9989E-01   3  9.9765E-01   4  9.8970E-01   5  9.9361E-01
  6  1.0261E+00   7  1.0652E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   24 iterations
  1  9.9973E-01   2  9.9989E-01   3  9.9765E-01   4  9.8970E-01   5  9.9361E-01
  6  1.0261E+00   7  1.0652E+00
```

```
  1  6.6805E-02   2 -4.4957E-02   3 -9.7558E-02   4 -6.3008E-02   5  6.3384E-02
  6  2.1372E-01   7 -2.7114E-02   8 -1.2155E-01   9  1.5012E-01  10  5.9940E-02
 11 -5.8435E-02  12  3.8935E-02  13 -1.0845E-01  14 -2.2928E-02  15 -7.7952E-03
 16 -8.4320E-04  17 -4.6850E-03  18  3.2980E-03  19 -3.5903E-03  20  4.8872E-02
 21 -1.3804E-02  22  2.5373E-02  23 -2.7745E-02  24 -7.5342E-03  25 -1.0836E-01

              THE SUM OF SQUARES IS   1.44421619E-01
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  C
FILE NAME: /SCREEN/:

          ================================================
          OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57:16

 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  25

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.01820942E+04    2.01874456E+04    2.01874456E+04    2.60519735E-02
 V2     -2.90936153E+01   -2.90969461E+01   -2.90969461E+01    1.41576514E-02
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     2.36701128E+04    2.37258699E+04    2.37258699E+04    1.00528933E-01
 V16    -7.56541588E+00   -7.64417506E+00   -7.64417506E+00    3.17218617E-01
 V17     3.00342393E+03    3.02274877E+03    3.02274877E+03    2.60675568E-01
 V19     2.20133191E+04    2.14534176E+04    2.14534176E+04    6.92924424E-01
 V20    -6.72498185E+00   -6.31333528E+00   -6.31333528E+00    1.79242658E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.51361771E-01 TO   1.44421619E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.02342328E-03

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.       10.      0.6680      6.6805E-02
1 W(LIQUID,B)=0.408              0.4071      2.00E-02 -8.9914E-04 -4.4957E-02
1 W(BCC#1,B)=0.13                0.1280      2.00E-02 -1.9512E-03 -9.7558E-02
2 T=1341                          1340.       10.     -0.6301     -6.3008E-02
2 HTR=3727                        3759.      5.00E+02   31.69      6.3384E-02
3 T=1049                          1051.       10.       2.137      0.2137
3 W(LIQUID,A)=0.27               0.2695      2.00E-02 -5.4229E-04 -2.7114E-02
3 W(BCC#1,A)=9.3E-2              9.0569E-02  2.00E-02 -2.4310E-03 -0.1216
5 T=726                           727.5       10.       1.501      0.1501
5 X(BCC#1,B)=3.7E-2              3.8199E-02  2.00E-02  1.1988E-03  5.9940E-02
5 X(BCC#2,A)=0.114               0.1128      2.00E-02 -1.1687E-03 -5.8435E-02
6 X(BCC#1,B)=3.7E-2              3.7779E-02  2.00E-02  7.7869E-04  3.8935E-02
6 X(BCC#2,A)=0.114               0.1118      2.00E-02 -2.1690E-03 -0.1085
10 W(LIQUID,A)=2E-2              1.9541E-02  2.00E-02 -4.5856E-04 -2.2928E-02
11 W(LIQUID,A)=4.2E-2            4.1844E-02  2.00E-02 -1.5590E-04 -7.7952E-03
12 W(LIQUID,A)=6.5E-2            6.4983E-02  2.00E-02 -1.6864E-05 -8.4320E-04
13 W(LIQUID,A)=9.3E-2            9.2906E-02  2.00E-02 -9.3701E-05 -4.6850E-03
20 W(LIQUID,A)=0.104             0.1041      2.00E-02  6.5960E-05  3.2980E-03
20 W(FCC,A)=3.8E-2               3.7928E-02  2.00E-02 -7.1806E-05 -3.5903E-03
21 W(LIQUID,A)=0.136             0.1370      2.00E-02  9.7745E-04  4.8872E-02
```

```
21 W(FCC,A)=4.7E-2              4.6724E-02  2.00E-02 -2.7608E-04 -1.3804E-02
22 W(LIQUID,A)=0.187            0.1875      2.00E-02  5.0746E-04  2.5373E-02
22 W(FCC,A)=5.9E-2              5.8445E-02  2.00E-02 -5.5490E-04 -2.7745E-02
23 W(LIQUID,A)=0.245            0.2448      2.00E-02 -1.5068E-04 -7.5342E-03
23 W(BCC#1,A)=8.5E-2            8.2833E-02  2.00E-02 -2.1672E-03 -0.1084

PARROT:
PARROT: @?<Hit_return_to_continue>
PARROT: @@ Calculate the phase diagram again
PARROT: mac tcex36cpd
PARROT: @@ The following commands are in the file tcex36cpd.TCM
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be runned in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          412  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
```

```
Generating start point   2
Generating start point   3
Generating start point   4
Generating start point   5
Generating start point   6
Generating start point   7
Generating start point   8
Generating start point   9
Generating start point  10
Working hard
Generating start point  11
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28

Phase region boundary   1 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..            2  equilibria
Terminating at axis limit.

Phase region boundary   2 at:   7.141E-01  3.000E+02
    BCC#1
 ** BCC#2
Calculated.            14  equilibria

Phase region boundary   3 at:   6.828E-01  7.275E+02
 ** A2B
    BCC#1
 ** BCC#2

Phase region boundary   4 at:   3.632E-01  7.275E+02
 ** A2B
    BCC#1
Calculated.            15  equilibria

      :
      :
      :

Phase region boundary  39 at:   6.122E-01  1.242E+03
    LIQUID
 ** A2B
Calculated.            13  equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.122E-01  1.242E+03
    LIQUID
 ** A2B
Calculated.             8  equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   9.927E-01  1.613E+03
    LIQUID
 ** FCC
Calculated.            20  equilibria
Terminating at known equilibrium

Phase region boundary  42 at:   9.927E-01  1.613E+03
```

```
    LIQUID
  ** FCC
 Calculated           12  equilibria
 *** BUFFER SAVED ON FILE: tcex36.POLY3
 CPU time for mapping           2  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
PLOTFILE : /SCREEN/:
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-inter
POST:
POST: @@ End of commands from tcex36cpd.TCM and back in tcex36b.TCM now
POST:
POST: @?<Hit_return_to_continue>
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid at high B
PARROT: @@ restore equilibrium 4 on the POP file
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read
   ... the command in full is READ_WORKSPACES
Block number /1/:  1
ED_EXP: s-e 4
   ... the command in full is SELECT_EQUILIBRIUM
 Equilibrium number            4 , label AINV
ED_EXP: s-we 1
   ... the command in full is SET_WEIGHT
Equilibria (range) or label(s) /PRESENT/:  PRESENT
ED_EXP: s-a-s
   ... the command in full is SET_ALL_START_VALUES
T /1204.671473/:  1200
Automatic start values for phase constituents? /N/:  N
 Phase LIQUID
Major constituent(s) /b/:  b
 Phase BCC
Major constituent(s) /b/:  b
 Phase FCC
Major constituent(s) /b/:  b
ED_EXP: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=1   FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1195.10 K (   921.95 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.29944E+02
 Total Gibbs energy -9.43347E+03,  Enthalpy  1.97100E+04,  Volume  0.00000E+00

 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
```

```
 A                      6.6854E-01  1.0290E-01 4.0783E-01 -8.9123E+03 SER
 B                      2.3315E+00  8.9710E-01 8.6070E-01 -1.4906E+03 SER

 FCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5876E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.40072E-01  A  5.99283E-02

 BCC#1                       Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5360E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.31812E-01  A  6.81875E-02

 LIQUID                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.8707E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.05502E-01  A  1.94498E-01

 EXPERIMENT T=1203:DT  $1195.1:10  NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX  $0.194498:2E-2  NO=2
 EXPERIMENT W(BCC#1,A)=6.9E-2:DX  $6.81875E-2:2E-2  NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX  $5.99283E-2:2E-2  NO=4
ED_EXP: @@ Now equilibrium 4 is on the high B side
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: ba
   ... the command in full is BACK
PARROT: resc
   ... the command in full is RESCALE_VARIABLES
PARROT: opt 0
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  C
FILE NAME: /SCREEN/:

           ================================================
           OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57:18

 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.01820942E+04    2.01820942E+04    2.01820942E+04    0.00000000E+00
 V2     -2.90936153E+01   -2.90936153E+01   -2.90936153E+01    0.00000000E+00
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     2.36701128E+04    2.36701128E+04    2.36701128E+04    0.00000000E+00
 V16    -7.56541588E+00   -7.56541588E+00   -7.56541588E+00    0.00000000E+00
 V17     3.00342393E+03    3.00342393E+03    3.00342393E+03    0.00000000E+00
 V19     2.20133191E+04    2.20133191E+04    2.20133191E+04    0.00000000E+00
 V20    -6.72498185E+00   -6.72498185E+00   -6.72498185E+00    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   8.21381872E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   3.73355396E-02

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
```

```
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.       10.      0.6680      6.6805E-02
1 W(LIQUID,B)=0.408              0.4071      2.00E-02 -8.9914E-04 -4.4957E-02
1 W(BCC#1,B)=0.13                0.1280      2.00E-02 -1.9512E-03 -9.7558E-02
2 T=1341                          1340.       10.     -0.6301     -6.3008E-02
2 HTR=3727                        3759.      5.00E+02   31.69      6.3384E-02
3 T=1049                          1051.       10.       2.137      0.2137
3 W(LIQUID,A)=0.27               0.2695      2.00E-02 -5.4229E-04 -2.7114E-02
3 W(BCC#1,A)=9.3E-2              9.0569E-02  2.00E-02 -2.4310E-03 -0.1216
4 T=1203                          1195.       10.      -7.904     -0.7904
4 W(LIQUID,A)=0.19               0.1945      2.00E-02  4.4978E-03  0.2249
4 W(BCC#1,A)=6.9E-2              6.8188E-02  2.00E-02 -8.1247E-04 -4.0623E-02
4 W(FCC,A)=6E-2                  5.9928E-02  2.00E-02 -7.1681E-05 -3.5840E-03
5 T=726                           727.5       10.       1.501      0.1501
5 X(BCC#1,B)=3.7E-2              3.8199E-02  2.00E-02  1.1988E-03  5.9940E-02
5 X(BCC#2,A)=0.114               0.1128      2.00E-02 -1.1687E-03 -5.8435E-02
6 X(BCC#1,B)=3.7E-2              3.7779E-02  2.00E-02  7.7869E-04  3.8935E-02
6 X(BCC#2,A)=0.114               0.1118      2.00E-02 -2.1690E-03 -0.1085
10 W(LIQUID,A)=2E-2              1.9541E-02  2.00E-02 -4.5856E-04 -2.2928E-02
11 W(LIQUID,A)=4.2E-2            4.1844E-02  2.00E-02 -1.5590E-04 -7.7952E-03
12 W(LIQUID,A)=6.5E-2            6.4983E-02  2.00E-02 -1.6864E-05 -8.4320E-04
13 W(LIQUID,A)=9.3E-2            9.2906E-02  2.00E-02 -9.3701E-05 -4.6850E-03
20 W(LIQUID,A)=0.104              0.1041      2.00E-02  6.5960E-05  3.2980E-03
20 W(FCC,A)=3.8E-2                3.7928E-02  2.00E-02 -7.1806E-05 -3.5903E-03
21 W(LIQUID,A)=0.136              0.1370      2.00E-02  9.7745E-04  4.8872E-02
21 W(FCC,A)=4.7E-2                4.6724E-02  2.00E-02 -2.7608E-04 -1.3804E-02
22 W(LIQUID,A)=0.187              0.1875      2.00E-02  5.0746E-04  2.5373E-02
22 W(FCC,A)=5.9E-2                5.8445E-02  2.00E-02 -5.5490E-04 -2.7745E-02
23 W(LIQUID,A)=0.245              0.2448      2.00E-02 -1.5068E-04 -7.5342E-03
23 W(BCC#1,A)=8.5E-2              8.2833E-02  2.00E-02 -2.1672E-03 -0.1084

PARROT:
PARROT: @?<Hit_return_to_continue>
PARROT: opt 30
   ... the command in full is OPTIMIZE_VARIABLES
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A

     AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    8.21381872E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    8.22200199E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

                         :
                         :
                         :

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.70124044E-01
  1  1.0007E+00   2  1.0004E+00   3  1.0050E+00   4  1.0192E+00   5  1.0109E+00
  6  1.0237E+00   7  1.0537E+00

     AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    1.67848298E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0074E+00   4  1.0249E+00   5  1.0142E+00
  6  1.0289E+00   7  1.0677E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   13 iterations
  1  1.0010E+00   2  1.0005E+00   3  1.0074E+00   4  1.0249E+00   5  1.0142E+00
  6  1.0289E+00   7  1.0677E+00

  1  6.3159E-02   2 -3.7855E-02   3 -8.1408E-02   4 -6.8333E-02   5  4.9922E-02
  6  2.5922E-01   7 -1.3945E-02   8 -9.1403E-02   9 -1.3190E-02  10  4.3921E-02
 11 -6.3821E-02  12 -8.0232E-02  13  1.6660E-01  14  3.1149E-02  15 -6.4318E-02
 16  8.0805E-03  17 -1.1993E-01  18 -1.7511E-02  19  4.0012E-04  20  7.0613E-03
 21 -6.1543E-04  22  4.9460E-03  23 -1.7570E-03  24  4.0977E-02  25 -2.3417E-02
 26 -2.5371E-03  27 -6.9022E-02  28  2.0311E-02  29 -7.1933E-02

              THE SUM OF SQUARES IS   1.67848298E-01
PARROT: l-r
```

```
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  C
FILE NAME: /SCREEN/:

          ================================================
          OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57:18

 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  14

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02022874E+04    2.01820942E+04    2.01820942E+04    2.48851184E-02
 V2     -2.91083471E+01   -2.90936153E+01   -2.90936153E+01    1.36092978E-02
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     2.38442466E+04    2.36701128E+04    2.36701128E+04    8.28181247E-02
 V16    -7.75413196E+00   -7.56541588E+00   -7.56541588E+00    2.55327523E-01
 V17     3.04598881E+03    3.00342393E+03    3.00342393E+03    2.36433676E-01
 V19     2.26500714E+04    2.20133191E+04    2.20133191E+04    4.73555900E-01
 V20    -7.18046350E+00   -6.72498185E+00   -6.72498185E+00    1.24878462E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.21381872E-01 TO   1.67848298E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   7.62946808E-03

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1194.       10.      0.6316      6.3159E-02
1 W(LIQUID,B)=0.408              0.4072      2.00E-02 -7.5710E-04 -3.7855E-02
1 W(BCC#1,B)=0.13                0.1284      2.00E-02 -1.6282E-03 -8.1408E-02
2 T=1341                          1340.       10.     -0.6833     -6.8333E-02
2 HTR=3727                        3752.      5.00E+02   24.96      4.9922E-02
3 T=1049                          1052.       10.       2.592      0.2592
3 W(LIQUID,A)=0.27               0.2697      2.00E-02 -2.7891E-04 -1.3945E-02
3 W(BCC#1,A)=9.3E-2              9.1172E-02  2.00E-02 -1.8281E-03 -9.1403E-02
4 T=1203                          1203.       10.     -0.1319     -1.3190E-02
4 W(LIQUID,A)=0.19               0.1909      2.00E-02  8.7843E-04  4.3921E-02
4 W(BCC#1,A)=6.9E-2              6.7724E-02  2.00E-02 -1.2764E-03 -6.3821E-02
4 W(FCC,A)=6E-2                  5.8395E-02  2.00E-02 -1.6046E-03 -8.0232E-02
5 T=726                           727.7       10.       1.666      0.1666
5 X(BCC#1,B)=3.7E-2              3.7623E-02  2.00E-02  6.2299E-04  3.1149E-02
5 X(BCC#2,A)=0.114               0.1127      2.00E-02 -1.2864E-03 -6.4318E-02
6 X(BCC#1,B)=3.7E-2              3.7162E-02  2.00E-02  1.6161E-04  8.0805E-03
6 X(BCC#2,A)=0.114               0.1116      2.00E-02 -2.3985E-03 -0.1199
10 W(LIQUID,A)=2E-2              1.9650E-02  2.00E-02 -3.5022E-04 -1.7511E-02
11 W(LIQUID,A)=4.2E-2            4.2008E-02  2.00E-02  8.0024E-06  4.0012E-04
12 W(LIQUID,A)=6.5E-2            6.5141E-02  2.00E-02  1.4123E-04  7.0613E-03
13 W(LIQUID,A)=9.3E-2            9.2988E-02  2.00E-02 -1.2309E-05 -6.1543E-04
20 W(LIQUID,A)=0.104             0.1041      2.00E-02  9.8920E-05  4.9460E-03
20 W(FCC,A)=3.8E-2               3.7965E-02  2.00E-02 -3.5141E-05 -1.7570E-03
21 W(LIQUID,A)=0.136             0.1368      2.00E-02  8.1954E-04  4.0977E-02
21 W(FCC,A)=4.7E-2               4.6532E-02  2.00E-02 -4.6833E-04 -2.3417E-02
22 W(LIQUID,A)=0.187             0.1869      2.00E-02 -5.0742E-05 -2.5371E-03
22 W(FCC,A)=5.9E-2                5.7620E-02  2.00E-02 -1.3804E-03 -6.9022E-02
23 W(LIQUID,A)=0.245              0.2454      2.00E-02  4.0621E-04  2.0311E-02
```

```
23 W(BCC#1,A)=8.5E-2            8.3561E-02  2.00E-02 -1.4387E-03 -7.1933E-02

PARROT:
PARROT: @?<Hit_return_to_continue>
PARROT: @@ Now optimize all parameters and all experiments
PARROT: l-a-v
   ... the command in full is LIST_ALL_VARIABLES
FILE NAME: /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02022874E+04    2.01820942E+04    2.01820942E+04    2.48851184E-02
 V2     -2.91083471E+01   -2.90936153E+01   -2.90936153E+01    1.36092978E-02
 V11    -2.18127453E+04
 V12     1.55559533E+01
 V15     2.38442466E+04    2.36701128E+04    2.36701128E+04    8.28181247E-02
 V16    -7.75413196E+00   -7.56541588E+00   -7.56541588E+00    2.55327523E-01
 V17     3.04598881E+03    3.00342393E+03    3.00342393E+03    2.36433676E-01
 V19     2.26500714E+04    2.20133191E+04    2.20133191E+04    4.73555900E-01
 V20    -7.18046350E+00   -6.72498185E+00   -6.72498185E+00    1.24878462E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.21381872E-01 TO   1.67848298E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   7.62946808E-03
PARROT: s-o-v 11-12
   ... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: ed
   ... the command in full is EDIT_EXPERIMENTS
ED_EXP: read
   ... the command in full is READ_WORKSPACES
Block number /1/:  1
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1193.6      LIQUID A2B BCC
   2 AINV   2   1.    1340.3      LIQUID A2B
   3 AINV   2   1.    1051.6      LIQUID A2B BCC
   4 AINV   2   1.    1202.9      LIQUID BCC FCC
   5 AINV   2   1.     727.7      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    2   1.    1594.0      LIQUID FCC
  11 ALF    2   1.    1548.0      LIQUID FCC
  12 ALF    2   1.    1499.0      LIQUID FCC
  13 ALF    2   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA   < unused >  1573.0      LIQUID
 101 AA   < unused >  1573.0      LIQUID
 102 AA   < unused >  1573.0      LIQUID
 103 AA   < unused >  1573.0      LIQUID
 104 AA   < unused >  1573.0      LIQUID
 105 AA   < unused >  1573.0      LIQUID
 106 AA   < unused >  1573.0      LIQUID
 107 AA   < unused >  1573.0      LIQUID
 108 AA   < unused >  1573.0      LIQUID
 110 AH   < unused >  1773.0      LIQUID
 111 AH   < unused >  1773.0      LIQUID
 112 AH   < unused >  1773.0      LIQUID
 113 AH   < unused >  1773.0      LIQUID
 114 AH   < unused >  1773.0      LIQUID
 115 AH   < unused >  1773.0      LIQUID
 116 AH   < unused >  1773.0      LIQUID
 117 AH   < unused >  1773.0      LIQUID
 118 AH   < unused >  1773.0      LIQUID
ED_EXP: s-we 1 100-118
   ... the command in full is SET_WEIGHT
ED_EXP: s-e 1
   ... the command in full is SELECT_EQUILIBRIUM
```

```
 Equilibrium number            1 , label AINV
ED_EXP: c-a
   ... the command in full is COMPUTE_ALL_EQUILIBRIA
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1193.6      LIQUID A2B BCC
   2 AINV   2   1.    1340.3      LIQUID A2B
   3 AINV   2   1.    1051.6      LIQUID A2B BCC
   4 AINV   2   1.    1202.9      LIQUID BCC FCC
   5 AINV   2   1.     727.7      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    2   1.    1594.0      LIQUID FCC
  11 ALF    2   1.    1548.0      LIQUID FCC
  12 ALF    2   1.    1499.0      LIQUID FCC
  13 ALF    2   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     2   1.    1773.0      LIQUID
 116 AH     2   1.    1773.0      LIQUID
 117 AH     2   1.    1773.0      LIQUID
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: save
   ... the command in full is SAVE_WORKSPACES
ED_EXP: ba
   ... the command in full is BACK
PARROT: opt
   ... the command in full is OPTIMIZE_VARIABLES
Number of iterations /30/:  30
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A

      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    5.15867048E-01
  1  1.0010E+00   2  1.0005E+00   3  1.0000E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    5.16671345E-01
  1  1.0011E+00   2  1.0005E+00   3  1.0000E+00   4  1.0000E+00   5  1.0074E+00
  6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

                         :
                         :
                         :

      AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    9.39274349E-02
  1  1.0066E+00   2  1.0086E+00   3  9.9812E-01   4  9.8393E-01   5  1.0177E+00
  6  1.0836E+00   7  1.0240E+00   8  1.0095E+00   9  1.0548E+00

      AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    6.73924414E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   16 iterations
  1  1.0093E+00   2  1.0115E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

  1 -5.7709E-02   2 -9.3404E-03   3  1.4435E-02   4  2.0965E-02   5 -2.5772E-02
  6 -5.2196E-02   7  1.9264E-02   8  2.6907E-02   9  1.1430E-02  10  2.7509E-02
 11  8.8335E-03  12  1.3391E-02  13 -4.8280E-02  14  2.2178E-02  15  5.2233E-03
```

```
 16  2.9006E-02  17  2.1915E-02  18 -2.1795E-02  19 -7.8107E-03  20 -4.4451E-03
 21 -1.5094E-02  22 -1.0366E-02  23  1.5822E-02  24  2.4683E-02  25  1.5219E-02
 26 -1.4822E-02  27  2.0406E-02  28 -1.2809E-02  29  1.5407E-02  30 -9.5946E-03
 31 -1.6846E-02  32  2.7408E-02  33  8.6976E-02  34  1.2428E-01  35  1.0162E-01
 36 -1.7386E-02  37  7.0520E-02  38 -1.9513E-02  39  1.6094E-02  40  4.5500E-02
 41  4.8219E-02  42  4.6251E-02  43  4.1594E-02  44  3.4251E-02  45  2.2219E-02
 46  7.5004E-03  47 -1.1906E-02

              THE SUM OF SQUARES IS   6.73924414E-02
PARROT: l-r
   ... the command in full is LIST_RESULT
FULL, CONDENSED OR GRAPHICAL FORMAT: /C/:  C
FILE NAME: /SCREEN/:

           ================================================
           OUTPUT FROM  P A R R O T.  DATE 2009. 4.29   15:57:18

 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  17

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820942E+04    2.01820942E+04    3.02498605E-02
 V2     -2.94290453E+01   -2.90936153E+01   -2.90936153E+01    2.30117884E-02
 V11    -2.17328114E+04   -2.18127453E+04   -2.18127453E+04    3.47139481E-02
 V12     1.52102756E+01    1.55559533E+01    1.55559533E+01    5.38555633E-02
 V15     2.42012671E+04    2.36701128E+04    2.36701128E+04    8.60925843E-02
 V16    -8.38545764E+00   -7.56541588E+00   -7.56541588E+00    2.83695193E-01
 V17     3.08774212E+03    3.00342393E+03    3.00342393E+03    2.37803043E-01
 V19     2.20600545E+04    2.20133191E+04    2.20133191E+04    4.87694952E-01
 V20    -7.07096154E+00   -6.72498185E+00   -6.72498185E+00    1.27666141E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15867048E-01 TO   6.73924414E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.77348530E-03

$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.       10.     -0.5771     -5.7709E-02
1 W(LIQUID,B)=0.408              0.4078      2.00E-02 -1.8681E-04 -9.3404E-03
1 W(BCC#1,B)=0.13                0.1303      2.00E-02  2.8870E-04  1.4435E-02
2 T=1341                          1341.       10.      0.2096      2.0965E-02
2 HTR=3727                        3714.      5.00E+02  -12.89     -2.5772E-02
3 T=1049                          1048.       10.     -0.5220     -5.2196E-02
3 W(LIQUID,A)=0.27               0.2704      2.00E-02  3.8528E-04  1.9264E-02
3 W(BCC#1,A)=9.3E-2              9.3538E-02  2.00E-02  5.3815E-04  2.6907E-02
4 T=1203                          1203.       10.      0.1143      1.1430E-02
4 W(LIQUID,A)=0.19               0.1906      2.00E-02  5.5017E-04  2.7509E-02
4 W(BCC#1,A)=6.9E-2              6.9177E-02  2.00E-02  1.7667E-04  8.8335E-03
4 W(FCC,A)=6E-2                  6.0268E-02  2.00E-02  2.6783E-04  1.3391E-02
5 T=726                           725.5       10.     -0.4828     -4.8280E-02
5 X(BCC#1,B)=3.7E-2              3.7444E-02  2.00E-02  4.4356E-04  2.2178E-02
5 X(BCC#2,A)=0.114               0.1141      2.00E-02  1.0447E-04  5.2233E-03
6 X(BCC#1,B)=3.7E-2              3.7580E-02  2.00E-02  5.8011E-04  2.9006E-02
6 X(BCC#2,A)=0.114               0.1144      2.00E-02  4.3830E-04  2.1915E-02
10 W(LIQUID,A)=2E-2              1.9564E-02  2.00E-02 -4.3589E-04 -2.1795E-02
```

```
11 W(LIQUID,A)=4.2E-2           4.1844E-02  2.00E-02 -1.5621E-04 -7.8107E-03
12 W(LIQUID,A)=6.5E-2           6.4911E-02  2.00E-02 -8.8903E-05 -4.4451E-03
13 W(LIQUID,A)=9.3E-2           9.2698E-02  2.00E-02 -3.0187E-04 -1.5094E-02
20 W(LIQUID,A)=0.104            0.1038      2.00E-02 -2.0732E-04 -1.0366E-02
20 W(FCC,A)=3.8E-2              3.8316E-02  2.00E-02  3.1644E-04  1.5822E-02
21 W(LIQUID,A)=0.136            0.1365      2.00E-02  4.9366E-04  2.4683E-02
21 W(FCC,A)=4.7E-2              4.7304E-02  2.00E-02  3.0438E-04  1.5219E-02
22 W(LIQUID,A)=0.187            0.1867      2.00E-02 -2.9645E-04 -1.4822E-02
22 W(FCC,A)=5.9E-2              5.9408E-02  2.00E-02  4.0813E-04  2.0406E-02
23 W(LIQUID,A)=0.245            0.2447      2.00E-02 -2.5617E-04 -1.2809E-02
23 W(BCC#1,A)=8.5E-2            8.5308E-02  2.00E-02  3.0814E-04  1.5407E-02
100 ACR(B)=0.94                 0.9397      2.85E-02 -2.7309E-04 -9.5946E-03
101 ACR(B)=0.84                 0.8395      2.82E-02 -4.7482E-04 -1.6846E-02
102 ACR(B)=0.74                 0.7408      2.81E-02  7.6893E-04  2.7408E-02
103 ACR(B)=0.64                 0.6424      2.81E-02  2.4411E-03  8.6976E-02
104 ACR(B)=0.54                 0.5435      2.82E-02  3.5079E-03  0.1243
105 ACR(B)=0.44                 0.4429      2.85E-02  2.9003E-03  0.1016
106 ACR(B)=0.34                 0.3395      2.90E-02 -5.0467E-04 -1.7386E-02
107 ACR(B)=0.23                 0.2321      2.97E-02  2.0948E-03  7.0520E-02
108 ACR(B)=0.12                 0.1194      3.06E-02 -5.9712E-04 -1.9513E-02
110 HMR(LIQUID)=-1964           -1956.      5.00E+02   8.047      1.6094E-02
111 HMR(LIQUID)=-3500           -3477.      5.00E+02   22.75      4.5500E-02
112 HMR(LIQUID)=-4588           -4564.      5.00E+02   24.11      4.8219E-02
113 HMR(LIQUID)=-5239           -5216.      5.00E+02   23.13      4.6251E-02
114 HMR(LIQUID)=-5454           -5433.      5.00E+02   20.80      4.1594E-02
115 HMR(LIQUID)=-5233           -5216.      5.00E+02   17.13      3.4251E-02
116 HMR(LIQUID)=-4575           -4564.      5.00E+02   11.11      2.2219E-02
117 HMR(LIQUID)=-3481           -3477.      5.00E+02   3.750      7.5004E-03
118 HMR(LIQUID)=-1950           -1956.      5.00E+02  -5.953     -1.1906E-02

PARROT:
PARROT: @?<Hit_return_to_continue>
PARROT: @@ Calculate the phase diagram a final time.
PARROT: mac tcex36cpd
PARROT: @@ The following commands are in the file tcex36cpd.TCM
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be runned in PARROT
PARROT: go p-3
   ... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
 *** WARNING *** Global equilibrium calculation may create new composition sets
 and this may corrupt your PARROT work file (.PAR file).
 Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition W(B)=.1234  created
POLY_3: s-a-v 2 t 300 1700,,,,
   ... the command in full is SET_AXIS_VARIABLE
 The condition T=942.2  created
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 W(B)=0.1234, P=1E5, N=1, T=500
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          412  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: save tcex36 y
   ... the command in full is SAVE_WORKSPACES
```

```
 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   7.140E-01  3.100E+02
     BCC#1
  ** BCC#2
 Calculated..            2  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   7.141E-01  3.000E+02
     BCC#1
  ** BCC#2
 Calculated.           14  equilibria

 Phase region boundary   3 at:   6.819E-01  7.255E+02
  ** A2B
     BCC#1
  ** BCC#2

 Phase region boundary   4 at:   3.626E-01  7.255E+02
  ** A2B
     BCC#1
 Calculated.           15  equilibria
```

```
      :
      :
      :

 Phase region boundary  39 at:   6.122E-01  1.240E+03
    LIQUID
  ** A2B
 Calculated.           14  equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.240E+03
    LIQUID
  ** A2B
 Calculated.            8  equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
    LIQUID
  ** FCC
 Calculated.           20  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
    LIQUID
  ** FCC
 Calculated            9  equilibria
 *** BUFFER SAVED ON FILE: tcex36.POLY3
 CPU time for mapping           2  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
PLOTFILE : /SCREEN/:
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: set-inter
POST:
POST: @@ End of commands from tcex36cpd.TCM and back in tcex36b.TCM now
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Add the experimental data
POST: a-e-d y tcex36
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  1
POST: plot
PLOTFILE : /SCREEN/:
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
   ... the command in full is BACK
POLY_3: read,,,
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-c t=1773
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         412  grid points in           0  s
 Found the set of lowest grid points in           0  s
```

```
 Calculated POLY solution       0 s, total time     0  s
POLY_3: sh hmr
   ... the command in full is SHOW_VALUE
 HMR=13116.476
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT              STATUS    REF. STATE     T(K)           P(Pa)
 A                      ENTERED   SER
 B                      ENTERED   SER
POLY_3: s-r-s a liq * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s b liq * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: save tcex36h y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value   0.123400
 Global calculation of initial equilibrium ....OK

 Phase Region from   0.123400     for:
     LIQUID
 Global test at  3.23400E-01 .... OK
 Global test at  5.73400E-01 .... OK
 Global test at  8.23400E-01 .... OK
 Global test at  9.53400E-01 .... OK
 Global test at  1.00000E+00 .... OK
 Terminating at    1.00000
 Calculated    51 equilibria

 Phase Region from   0.123400     for:
     LIQUID
 Global test at  8.34000E-02 .... OK
 Global test at  3.34000E-02 .... OK
 Terminating at   0.250000E-11
 Calculated    28 equilibria
 *** Buffer saved on file: tcex36h.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

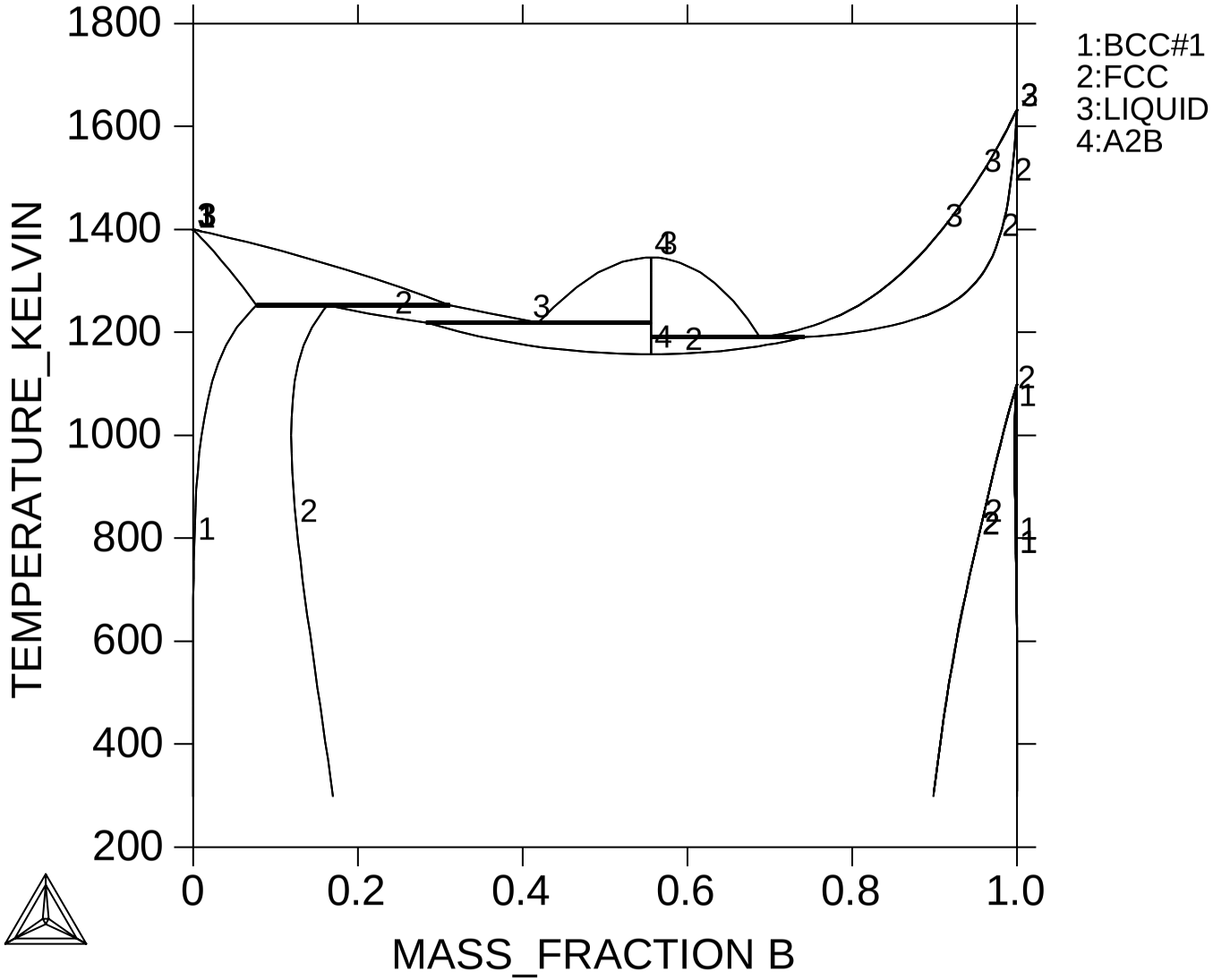
POST:
POST:
POST: s-d-a x x(b)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y hmr(liq)
   ... the command in full is SET_DIAGRAM_AXIS
POST: a-e-d y tcex36
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  2
POST: plot
PLOTFILE : /SCREEN/:
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: ba
   ... the command in full is BACK
```

```
 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-result gra tcex36-dia
   ... the command in full is LIST_RESULT
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: go p-3
  No such command, use HELP
POST: read,,
  No such command, use HELP
POST: post
  No such command, use HELP
POST: q tcex36-dia.exp 1; 1;
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
POST:
POST:
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
```

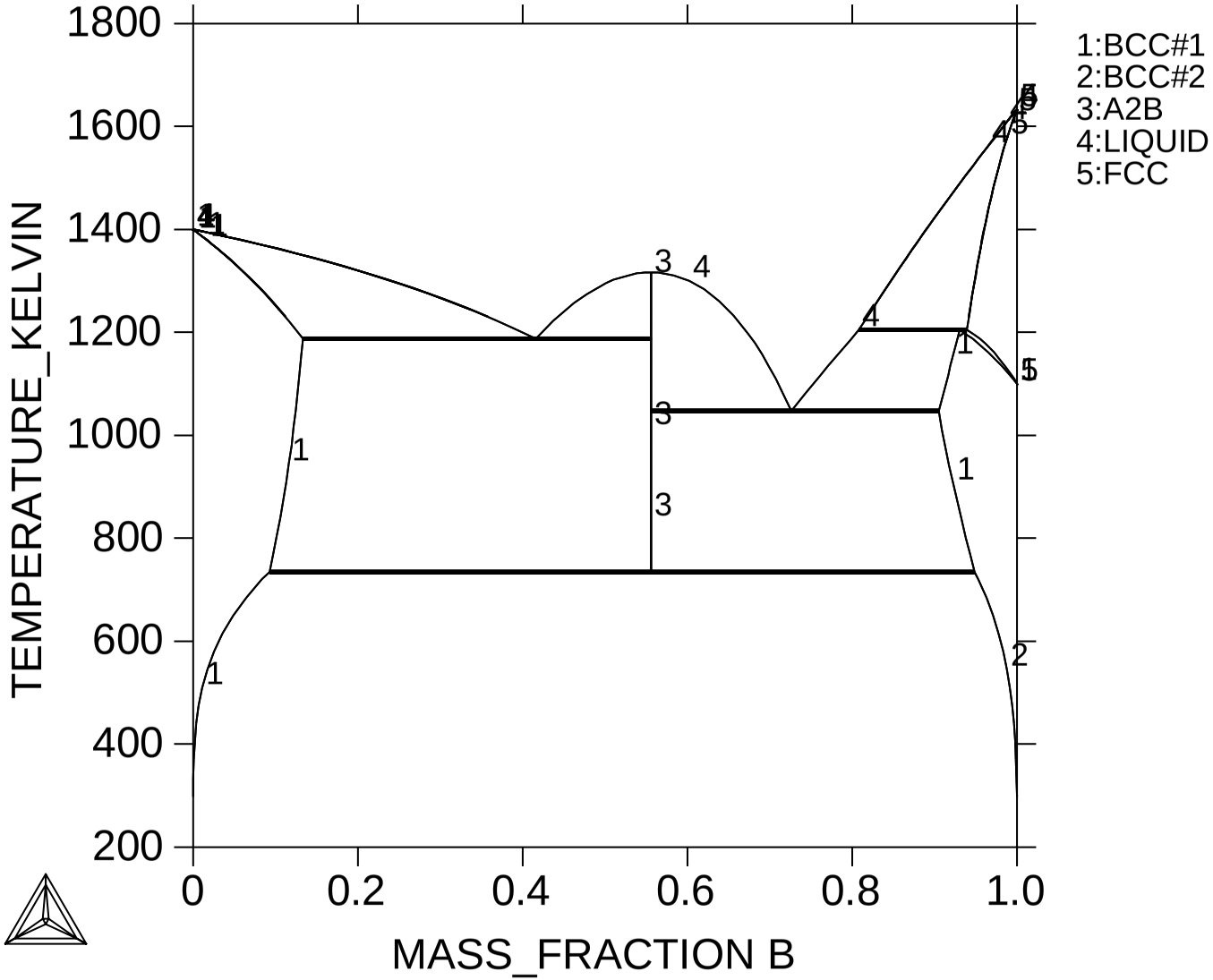
THERMO-CALC (2009.04.29:15.57) :

P=1E5, N=1



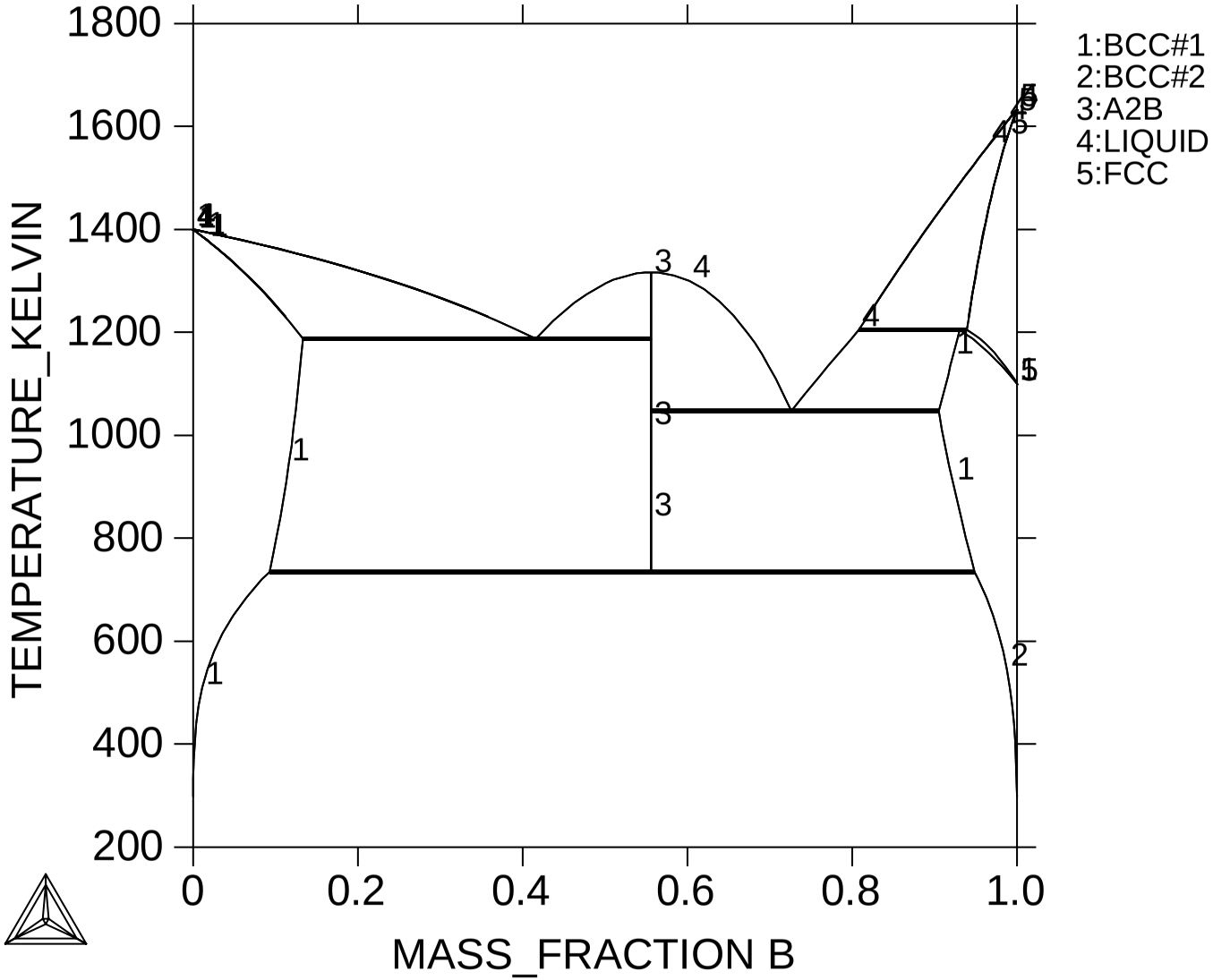
THERMO-CALC (2009.04.29:15.57) :

P=1E5, N=1



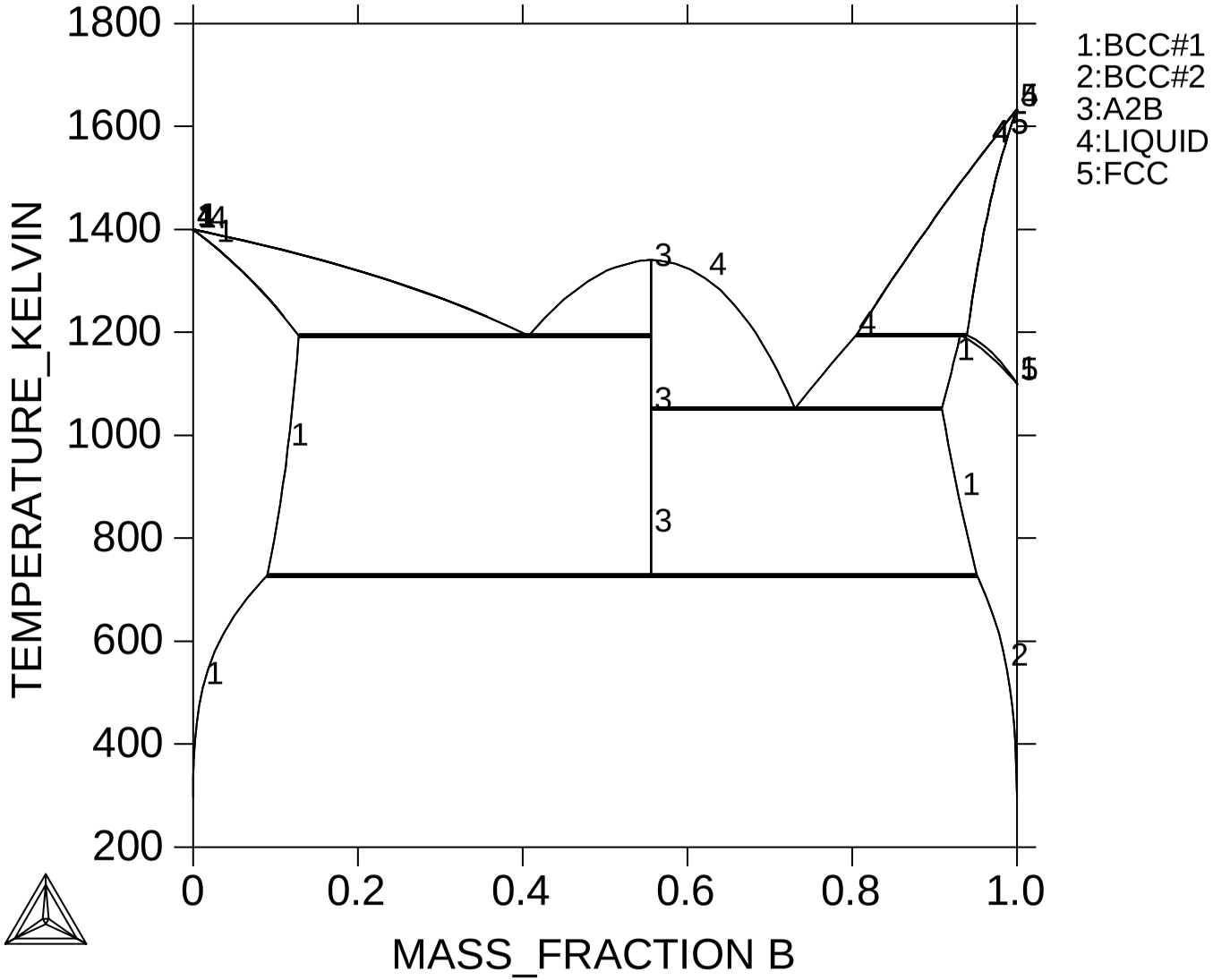
THERMO-CALC (2009.04.29:15.57) :

P=1E5, N=1



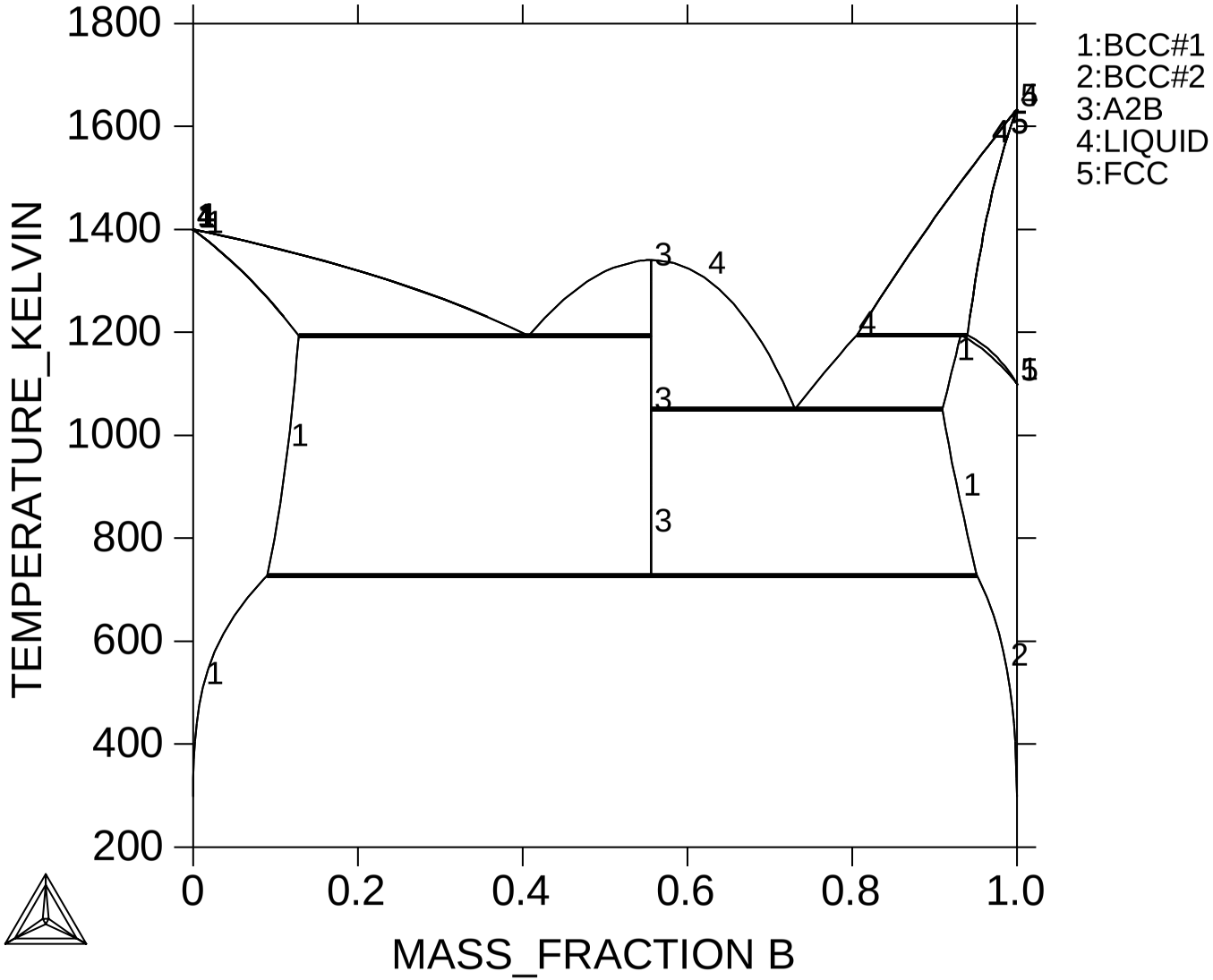
THERMO-CALC (2009.04.29:15.57) :

P=1E5, N=1



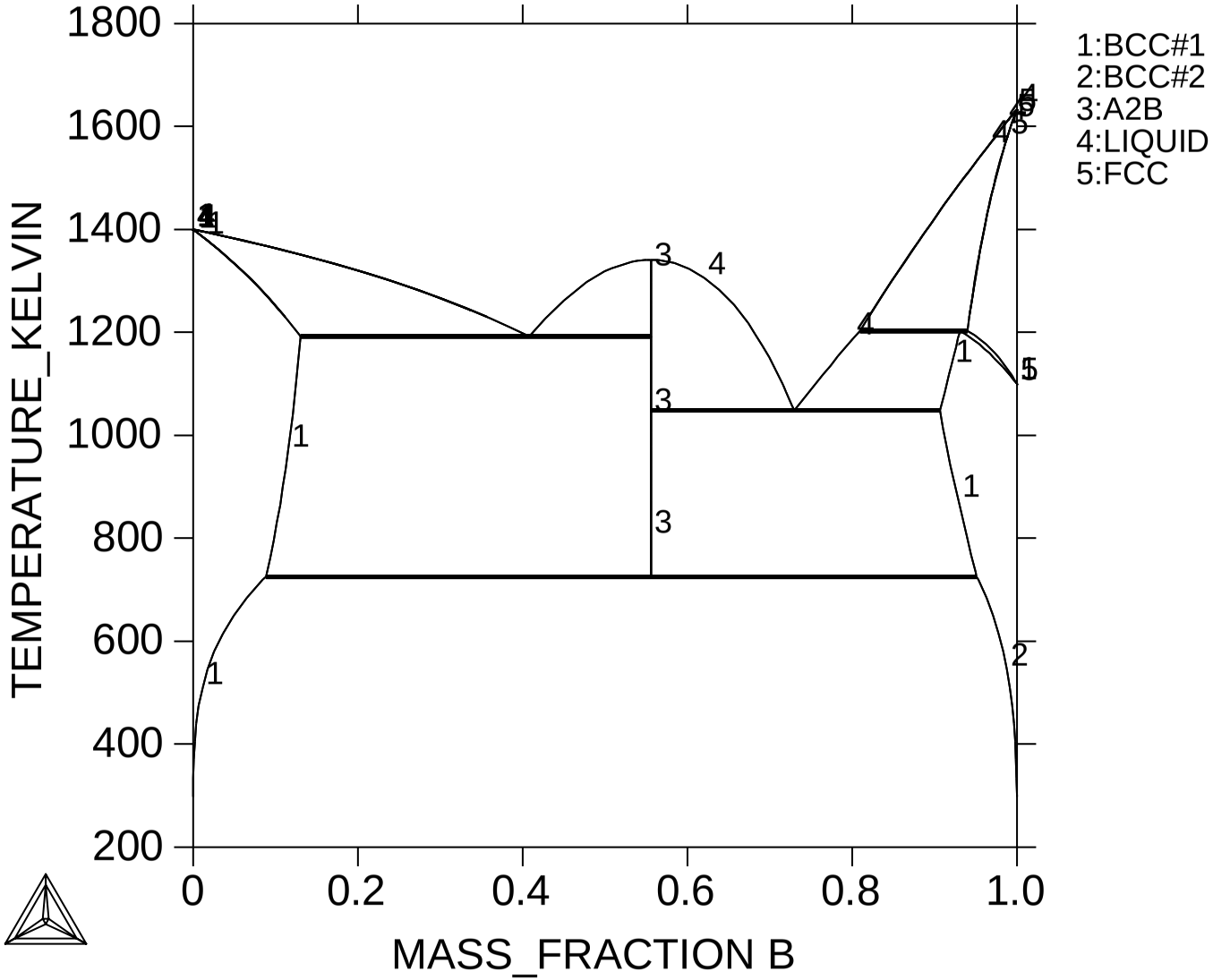
THERMO-CALC (2009.04.29:15.57) :

P=1E5, N=1



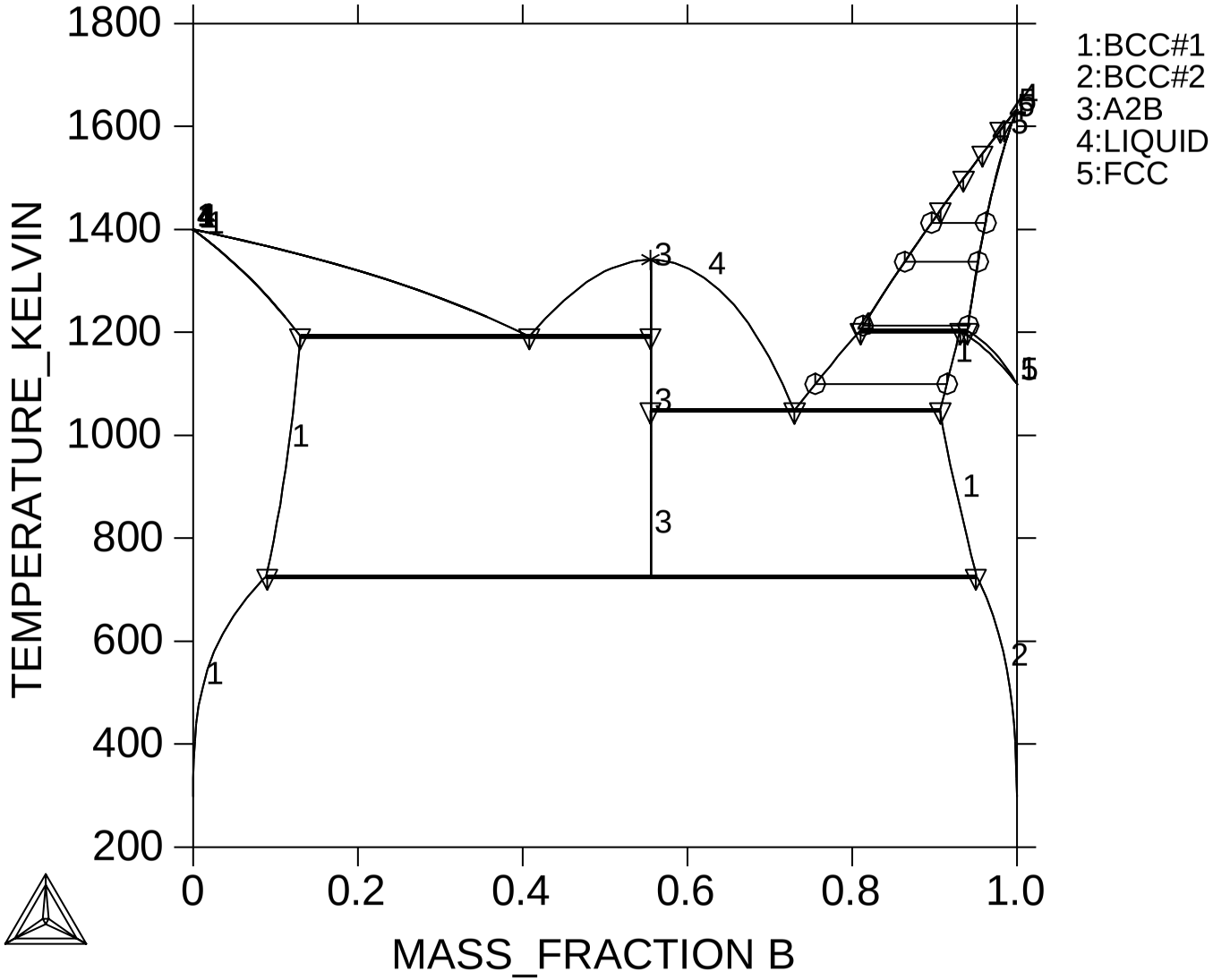
THERMO-CALC (2009.04.29:15.57) :

P=1E5, N=1



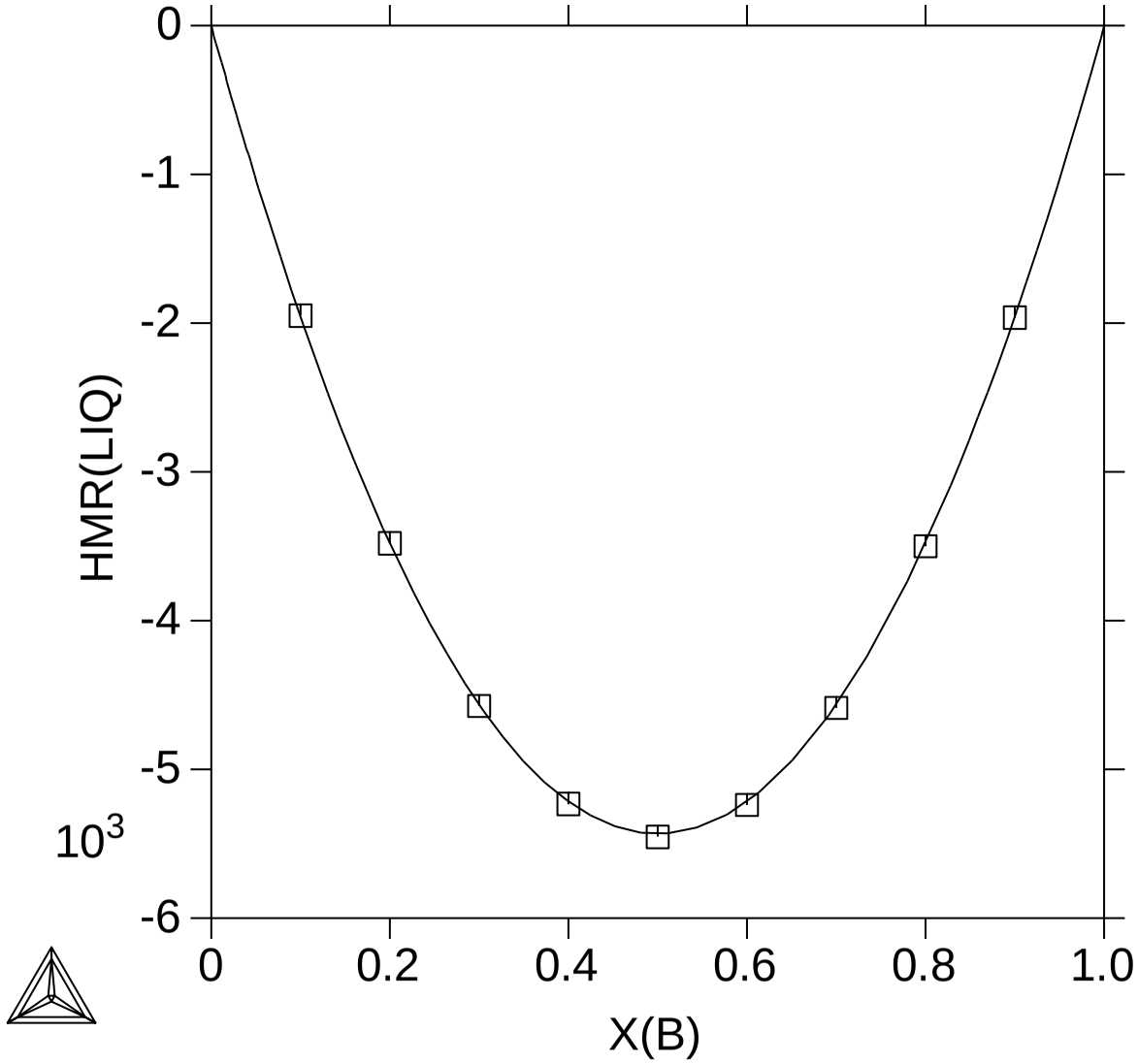
THERMO-CALC (2009.04.29:15.57) :

P=1E5, N=1

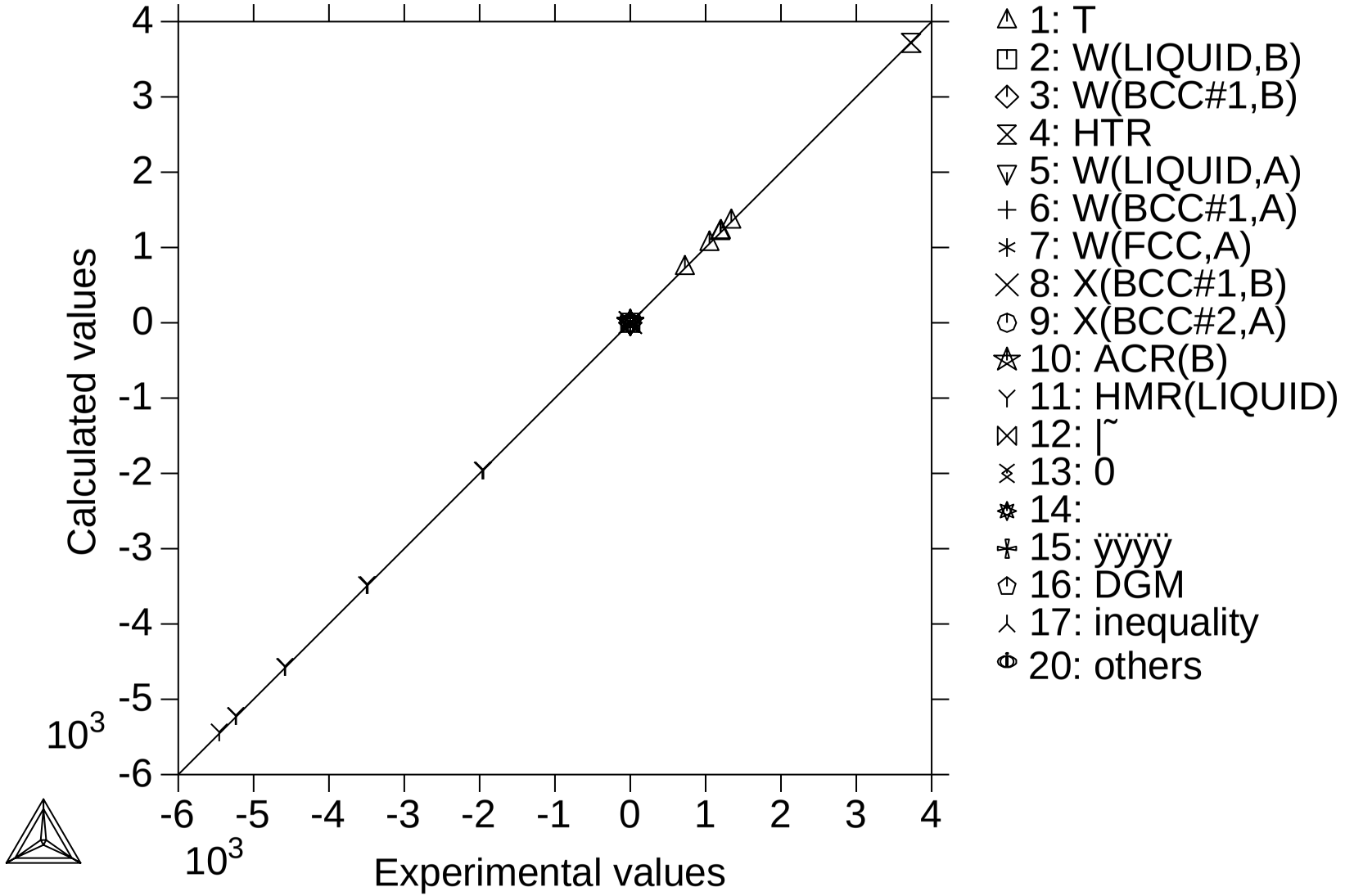


THERMO-CALC (2009.04.29:15.57) :

P=1E5, N=1, T=1773;



THERMO-CALC (2009.04.29:15.57) : From PARROT optimization



37

Calculation of an isothermal section

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of an isothermal section, using command-lines
SYS: @@
SYS: set-log tcex37,,
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw pkp
   ... the command in full is SWITCH_DATABASE
 Current database: Kaufman Binary Alloys TDB v1

TDB_PKP: def-sys
   ... the command in full is DEFINE_SYSTEM
ELEMENTS: fe cr ni
 FE                      CR                      NI
   DEFINED
TDB_PKP: l-s c
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :CR FE NI:
 BCC         :CR FE NI:
 FCC         :CR FE NI:
 HCP         :CR FE NI:
 RHOMBOHEDRAL :CR FE NI:
 ALPHA_MN    :FE:
 BETHA_MN    :FE:
 SIGMA_CRFE  :CR:FE:
 FENI3       :FE:NI:
TDB_PKP: rej ph /?
   ... the command in full is REJECT
To be REJECTED: LIQUID:L  No/Quit/* /Yes/: n
To be REJECTED: BCC  No/Quit/* /Yes/: n
To be REJECTED: FCC  No/Quit/* /Yes/: n
To be REJECTED: HCP  No/Quit/* /Yes/: yes
To be REJECTED: RHOMBOHEDRAL  No/Quit/* /Yes/: yes
To be REJECTED: ALPHA_MN  No/Quit/* /Yes/: yes
To be REJECTED: BETHA_MN  No/Quit/* /Yes/: yes
To be REJECTED: SIGMA_CRFE  No/Quit/* /Yes/: n
To be REJECTED: FENI3  No/Quit/* /Yes/: n
TDB_PKP: l-s,,
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :CR FE NI:
 BCC         :CR FE NI:
 FCC         :CR FE NI:
 SIGMA_CRFE  :CR:FE:
 FENI3       :FE:NI:
TDB_PKP: @?<Hit_return_to_continue>
TDB_PKP: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_PKP: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: l-st
```

```
   ... the command in full is LIST_STATUS
Option /CPS/: cps
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 NI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 SIGMA_CRFE              ENTERED    0.00000000E+00  0.00000000E+00
 FENI3                   ENTERED    0.00000000E+00  0.00000000E+00
 FCC                     ENTERED    0.00000000E+00  0.00000000E+00
 BCC                     ENTERED    0.00000000E+00  0.00000000E+00
 LIQUID                  ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 CR ENTERED    FE ENTERED    NI ENTERED
POLY_3: @@ Set conditions for a point inside the diagram
POLY_3: s-c x(cr)=0.2 x(ni)=0.4
   ... the command in full is SET_CONDITION
POLY_3: s-c t=1673 p=1e5 n=1
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 X(CR)=0.2, X(NI)=0.4, T=1673, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         5933  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: PKP

 Conditions:
 X(CR)=0.2, X(NI)=0.4, T=1673, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1673.00 K (  1399.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.62140E+01
 Total Gibbs energy -1.54502E+04,  Enthalpy  1.98718E+03,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      2.0000E-01  1.8499E-01 2.7994E-01 -1.7710E+04 SER
 FE                      4.0000E-01  3.9739E-01 4.0576E-01 -1.2547E+04 SER
 NI                      4.0000E-01  4.1762E-01 2.8991E-01 -1.7223E+04 SER

 FCC                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.6214E+01, Volume fraction 0.0000E+00  Mass fractions:
 NI  4.17618E-01  FE  3.97389E-01  CR  1.84993E-01
POLY_3: s-a-v
   ... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: s-a-v 2
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: x(cr)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: save tcex37 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
```

```
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Working hard
 Generating start point   1
 Generating start point   2
 ERROR         1611  when calculating equilibrium
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 ERROR         1611  when calculating equilibrium
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Working hard

 Phase region boundary   1 at:   8.908E-03  1.694E-02
  ** BCC
     FCC
 *** Buffer saved on file: tcex37.POLY3
 Calculated           17  equilibria

 Phase region boundary   2 at:   8.908E-03  1.694E-02
  ** BCC
     FCC
 Calculated.           24  equilibria

 Phase region boundary   3 at:   1.087E-01  3.133E-01
  ** LIQUID
  ** BCC
     FCC

 Phase region boundary   4 at:   1.465E-01  2.894E-01
  ** LIQUID
     FCC
 Calculated           55  equilibria

       :
       :
       :

 Phase region boundary  11 at:   1.594E-01  5.916E-01
  ** LIQUID
     BCC
 Calculated.           22  equilibria
 Terminating at known equilibrium

 Phase region boundary  12 at:   1.594E-01  5.916E-01
  ** LIQUID
     BCC
 Calculated           37  equilibria

 Phase region boundary  13 at:   2.987E-01  6.929E-01
     LIQUID
  ** BCC
 Calculated           20  equilibria

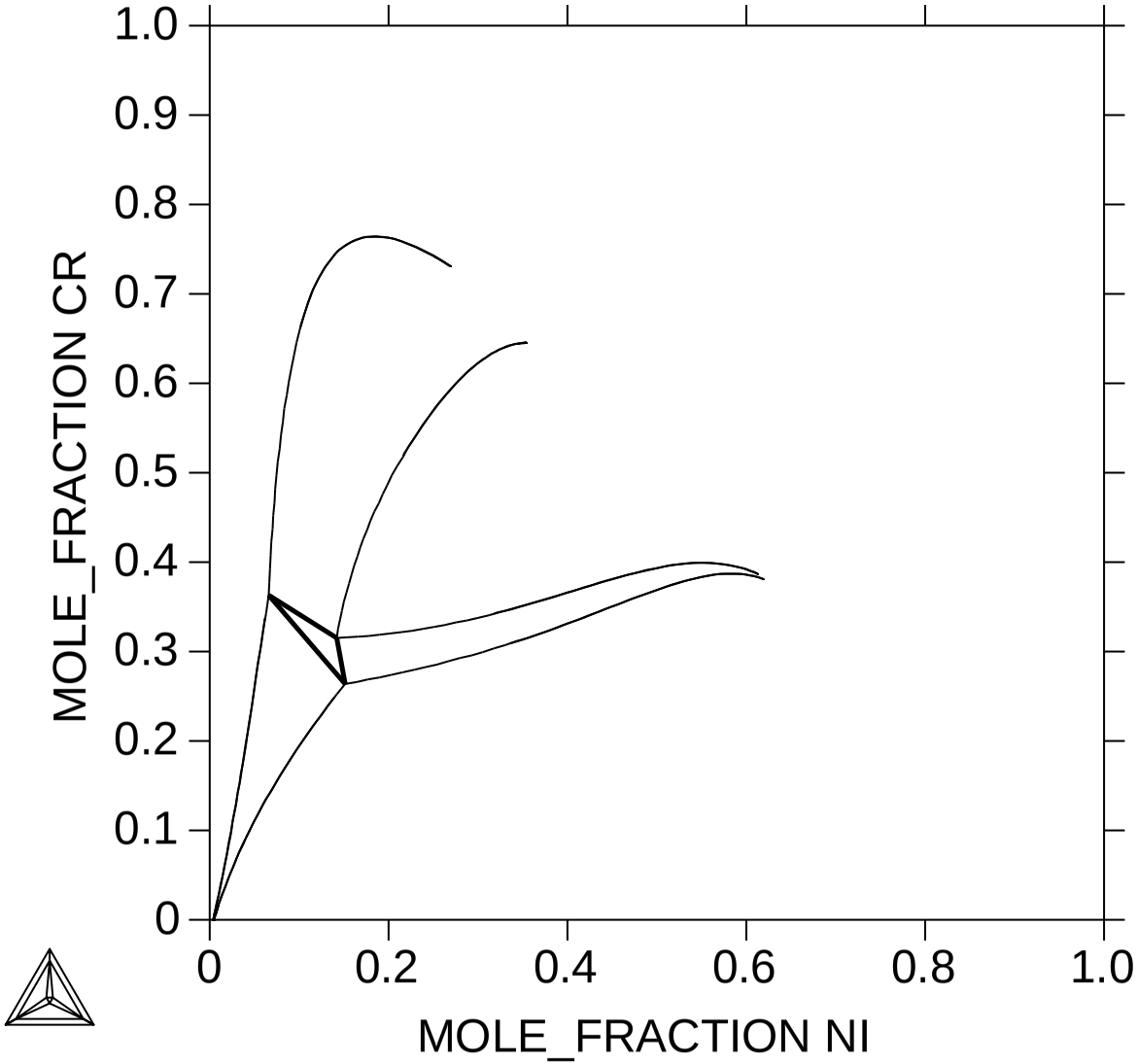
 Phase region boundary  14 at:   2.987E-01  6.929E-01
     LIQUID
  ** BCC
 Calculated.           42  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex37.POLY3
```

```
 CPU time for mapping           3  seconds
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

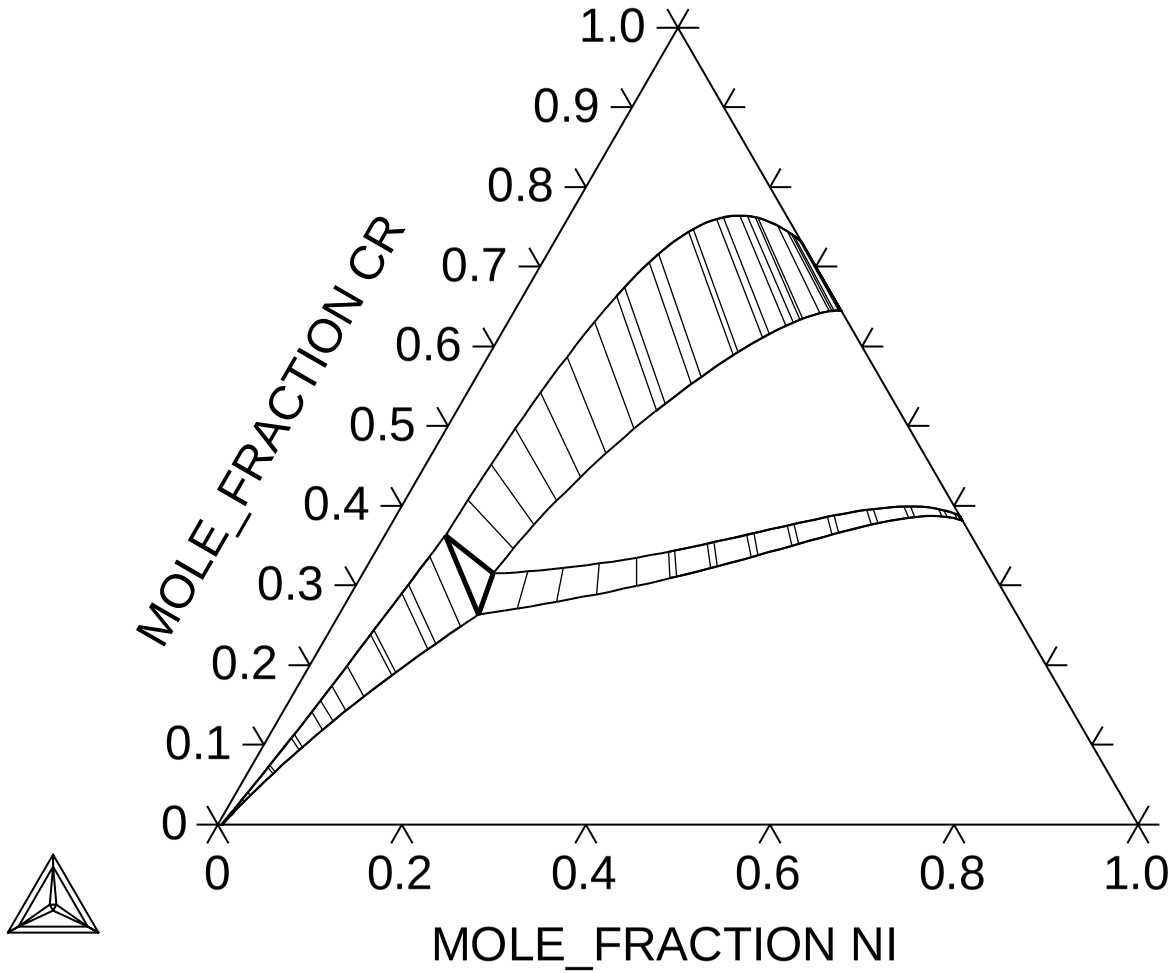
 Setting automatic diagram axis

POST: @@ Use default axis on the diagram
POST:
POST: set-title example 37a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ By default a diagram is always square. set it triangular,
POST: @@ add tie-lines and set scaling on the axis
POST: s-d-t
   ... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM  (Y OR N) /N/:  y
PLOT 3:RD AXIS  (Y OR N) /Y/:  y
CLIP ALONG 3:RD AXIS  (Y OR N) /Y/:  y
POST: s-t-s
   ... the command in full is SET_TIELINE_STATUS
PLOTTING EVERY TIE-LINE NO /0/:  3
POST: s-sc
   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING  (Y OR N) /N/:  n
MIN VALUE : 0
MAX VALUE : 1
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 37b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ To identify the phases also set labels
POST: @@ To add text in phase regions use a dataplot file
POST: set-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 37c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           3  seconds
```

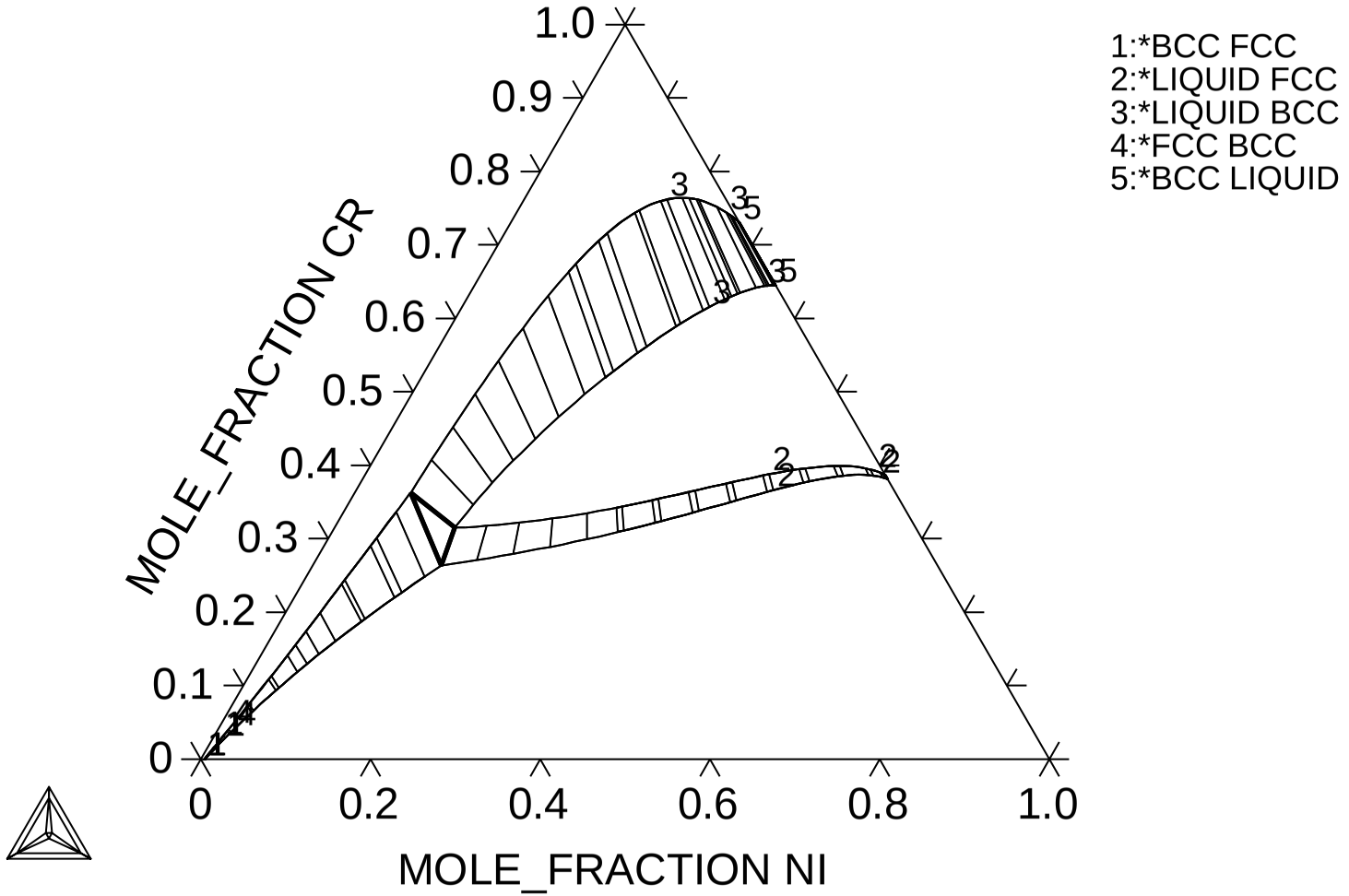
THERMO-CALC (2009.04.15:03.09) :example 37a
DATABASE:PKP
T=1673, P=1E5, N=1;



THERMO-CALC (2009.04.15:03.09) :example 37b
DATABASE:PKP
T=1673, P=1E5, N=1;



THERMO-CALC (2009.04.15:03.09) :example 37c
DATABASE:PKP
T=1673, P=1E5, N=1;



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Calculation of the Morral "rose"

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of miscibility gaps ...
SYS: @@
SYS: set-log ex38,,,,
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
 First version released 1-Jan-78, last update 20-Nov-2007

GES: rei,,,,,,
   ... the command in full is REINITIATE
GES:
GES: @@ Enter a phase with just a ternary interaction parameter
GES: e-e a b c
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
GES: a-e-d a fcc 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d b fcc 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d c fcc 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES:
GES:
GES: e-ph fcc,,1 A B C;,,,,,
   ... the command in full is ENTER_PHASE
GES:
GES:
GES: e-par l(fcc,a,b,c),,50000;,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC,A,B,C;0)
GES: l-d
   ... the command in full is LIST_DATA
OUTPUT FILE: /SCREEN/:
OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH           DATE 2009- 4-15
 FROM DATABASE: User data 2009. 4.15

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  1 A    FCC                      1.0000E+01  0.0000E+00  0.0000E+00
  2 B    FCC                      1.0000E+01  1.2220E+03  5.9000E+00
  3 C    FCC                      1.0000E+01  1.0540E+03  5.7400E+00

 SPECIES                                  STOICHIOMETRY
   1 A                                    A
   2 B                                    B
   3 C                                    C

 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B,C

      G(FCC,A;0)-G(FCC,A;0) = 0.0
      G(FCC,B;0)-G(FCC,B;0) = 0.0
      G(FCC,C;0)-G(FCC,C;0) = 0.0
      L(FCC,A,B,C;0) = 50000
```

```
 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)

GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3:
POLY_3: s-c t=600 p=1e5 n=1 x(b)=.3 x(c)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Creating a new composition set FCC#2
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=600, P=1E5, N=1, X(B)=0.3, X(C)=0.1
 DEGREES OF FREEDOM 0

 Temperature    600.00 K (   326.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.58989E+03,  Enthalpy  6.74567E+02,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 5.7356E-01 -2.7732E+03 SER
 B                       3.0000E-01  3.0000E-01 3.8092E-01 -4.8149E+03 SER
 C                       1.0000E-01  1.0000E-01 3.8092E-01 -4.8149E+03 SER

 FCC#1                       Status ENTERED     Driving force  0.0000E+00
 Moles 8.7781E-01, Mass 8.7781E+00, Volume fraction 0.0000E+00  Mass fractions:
 A  6.00000E-01  B  3.32342E-01  C  6.76579E-02

 FCC#2                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.2219E-01, Mass 1.2219E+00, Volume fraction 0.0000E+00  Mass fractions:
 A  6.00000E-01  C  3.32342E-01  B  6.76579E-02
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-a-v 1 x(b) 0 1 0.01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(c) 0 1 0.01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: save tcex38 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Trying global minimization! 3
 Generating start point   1
 Generating start point   2
 Trying global minimization! 3
```

```
 Generating start point   3
 Generating start point   4
 ERROR         1611  when calculating equilibrium
 Trying global minimization! 3
 Creating a new composition set FCC#3
 Generating start point   5
 Generating start point   6
 Trying global minimization! 3
 Generating start point   7
 Generating start point   8
 Trying global minimization! 3
 Generating start point   9
 Generating start point  10
 Working hard
 Trying global minimization! 3
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14

 Phase region boundary   1 at:   9.900E-01  1.000E-02
     FCC#1
  ** FCC#2
 *** Buffer saved on file: tcex38.POLY3

 Phase region boundary   2 at:   9.900E-01  1.000E-02
     FCC#1
  ** FCC#2

 Phase region boundary   3 at:   2.333E-01  2.333E-01
     FCC#1
  ** FCC#2
 Calculated           35  equilibria
  ..
  ..
  ..
 Phase region boundary  22 at:   6.633E-01  1.683E-01
     FCC#1
  ** FCC#2
 Calculated           26  equilibria

 Phase region boundary  23 at:   6.633E-01  1.683E-01
     FCC#1
  ** FCC#2
 Calculated           33  equilibria

 Phase region boundary  24 at:   6.633E-01  1.683E-01
     FCC#1
  ** FCC#2
 Calculated.           22  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex38.POLY3
 CPU time for mapping           5  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,,
POST:
POST: s-d-a x m-f b
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y m-f c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
```

```
POST: s-t-s 10
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 38a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
 The composition set FCC#4 created from the store file
POST:
POST: @?<Hit_return_to_continue>
POST: back
POLY_3: read,,
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: @@ We will calculate at a higher temperature
POLY_3: @@ with a stable phase in the middle.
POLY_3: s-c t=696
   ... the command in full is SET_CONDITION
POLY_3: s-c x(b)=.44 x(c)=.28
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: save tcex38b y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Working hard
 Trying global minimization! 3
 Generating start point   1
 Generating start point   2
 ERROR         1611  when calculating equilibrium
 Trying global minimization! 3
 Generating start point   3
 Generating start point   4
 Trying global minimization! 3
 Generating start point   5
 Generating start point   6

 Phase region boundary   1 at:   2.683E-01  2.683E-01
     FCC#1
  ** FCC#2
 Calculated           35  equilibria

 Phase region boundary   2 at:   2.683E-01  2.683E-01
     FCC#1
  ** FCC#2
 Creating a new composition set FCC#3
 Calculated            6  equilibria

 Phase region boundary   3 at:   2.683E-01  2.683E-01
     FCC#1
  ** FCC#2
 Calculated            6  equilibria
  ..
```

```
  ..
  ..
 Phase region boundary  31 at:   2.683E-01  4.633E-01
     FCC#1
  ** FCC#2
 Calculated            9  equilibria

 Phase region boundary  32 at:   2.683E-01  4.633E-01
     FCC#1
  ** FCC#2
 Calculated.            9  equilibria
 Terminating at known equilibrium

 Phase region boundary  33 at:   2.683E-01  4.633E-01
     FCC#1
  ** FCC#2
 Calculated           41  equilibria
 *** BUFFER SAVED ON FILE: tcex38b.POLY3
 CPU time for mapping           4  seconds
POLY_3:
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,,
POST:
POST:
POST: set-title example 38b
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
 The composition set FCC#4 created from the store file
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: back
POLY_3: @@ ========================================
POLY_3: @@ Now a quaternary!
POLY_3: @@
POLY_3: @@ Square rose by John Morral
POLY_3: @@
POLY_3: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
GES: rei,,,,,
   ... the command in full is REINITIATE
GES: e-e a b c d
   ... the command in full is ENTER_ELEMENT
GES: a-e-d a liq 10,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d b liq 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d c liq 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d d liq 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: e-ph liquid
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/:  1
NAME OF CONSTITUENT: A B C D
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/:  NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/:  NO
GES: e-par g(liq,a,b,c,d)
```

```
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A,B,C,D;0)
LOW TEMPERATURE LIMIT /298.15/:  298.15
FUNCTION: 100000
&
HIGH TEMPERATURE LIMIT /6000/:  6000
ANY MORE RANGES /N/:  N
GES:
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: rei,,,,
   ... the command in full is REINITIATE_MODULE
POLY_3: s-c t=170 p=1e5 n=1 x(d)=.25 x(a)=.3 x(a)+x(c)=.5
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=170, P=1E5, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         1819  grid points in            0  s
 Creating a new composition set LIQUID#2
    32 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VXCS
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=170, P=1E5, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
 DEGREES OF FREEDOM 0

 Temperature    170.00 K (  -103.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -1.58399E+03,  Enthalpy  2.18612E+02,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       3.0000E-01  3.0000E-01 3.1587E-01 -1.6289E+03 SER
 B                       2.5000E-01  2.5000E-01 2.9182E-01 -1.7409E+03 SER
 C                       2.0000E-01  2.0000E-01 3.5423E-01 -1.4669E+03 SER
 D                       2.5000E-01  2.5000E-01 3.5423E-01 -1.4669E+03 SER

 LIQUID#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 5.8530E-01, Mass 5.8530E+00, Volume fraction 0.0000E+00  Mole fractions:
 D  3.71549E-01  A  3.00000E-01  B  2.50000E-01  C  7.84507E-02

 LIQUID#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 4.1470E-01, Mass 4.1470E+00, Volume fraction 0.0000E+00  Mole fractions:
 C  3.71549E-01  A  3.00000E-01  B  2.50000E-01  D  7.84507E-02
POLY_3: s-a-v 1 x(a)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  .5
Increment /.0125/:  .01
POLY_3: s-a-v 2 x(d)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  0
Max value /1/:  .5
Increment /.0125/:  .01
POLY_3:
POLY_3: add +1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: save tcex38c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
```

```
 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.478E-01  2.500E-01
     LIQUID#1
  ** LIQUID#2
 Creating a new composition set LIQUID#3
 Calculated           45  equilibria

 Phase region boundary   2 at:   4.478E-01  2.500E-01
     LIQUID#1
  ** LIQUID#2
 Calculated.           41  equilibria

 Phase region boundary   3 at:   2.500E-01  5.217E-02
     LIQUID#1
  ** LIQUID#2
  ** LIQUID#3
  ..
  ..
  ..
 Phase region boundary  27 at:   4.478E-01  2.500E-01
     LIQUID#1
  ** LIQUID#2
 Calculated            2  equilibria

 Phase region boundary  28 at:   4.478E-01  2.500E-01
     LIQUID#1
  ** LIQUID#2
 Calculated           24  equilibria

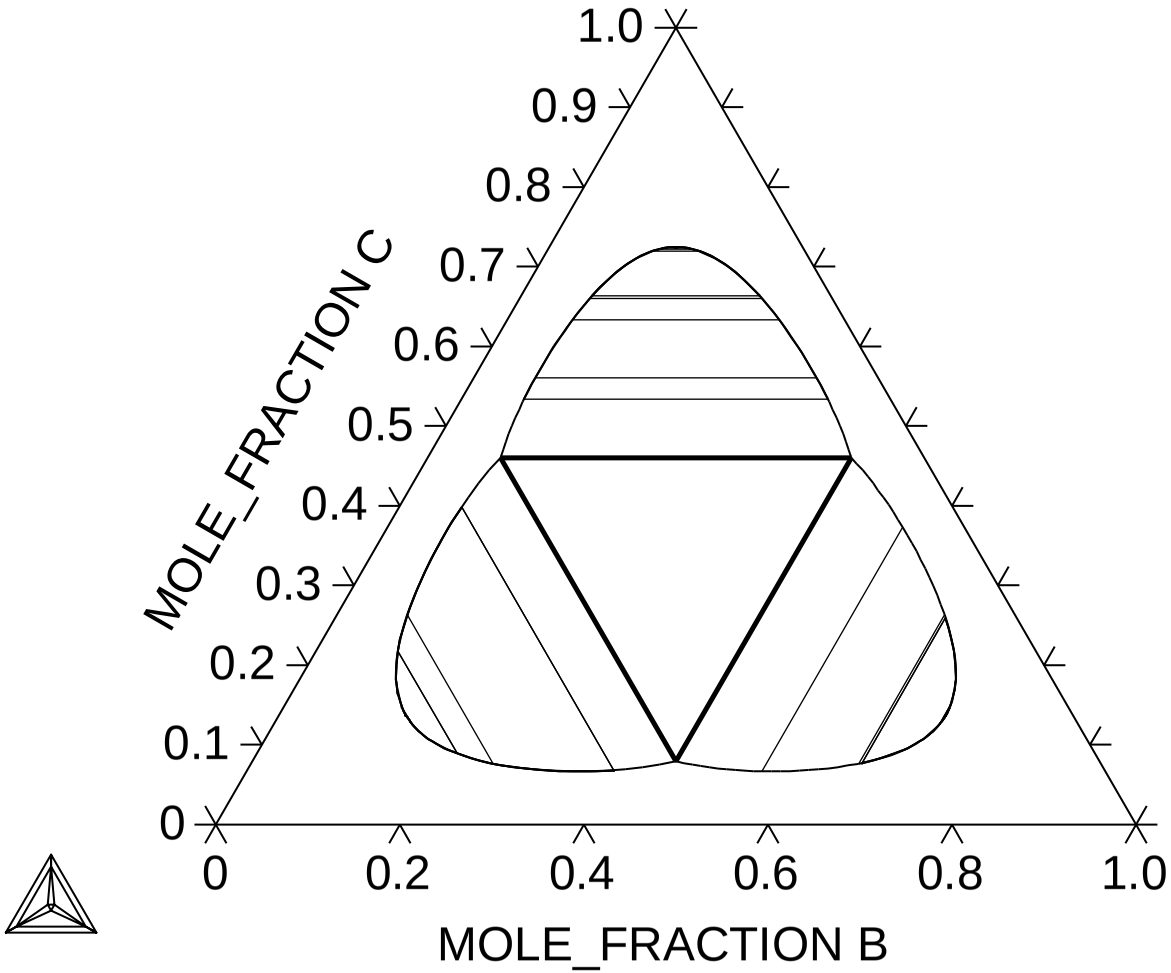
 Phase region boundary  29 at:   4.478E-01  2.500E-01
     LIQUID#1
  ** LIQUID#2
 Calculated            2  equilibria
 Calculated            2  equilibria
 *** BUFFER SAVED ON FILE: tcex38c.POLY3
 CPU time for mapping           4  seconds
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

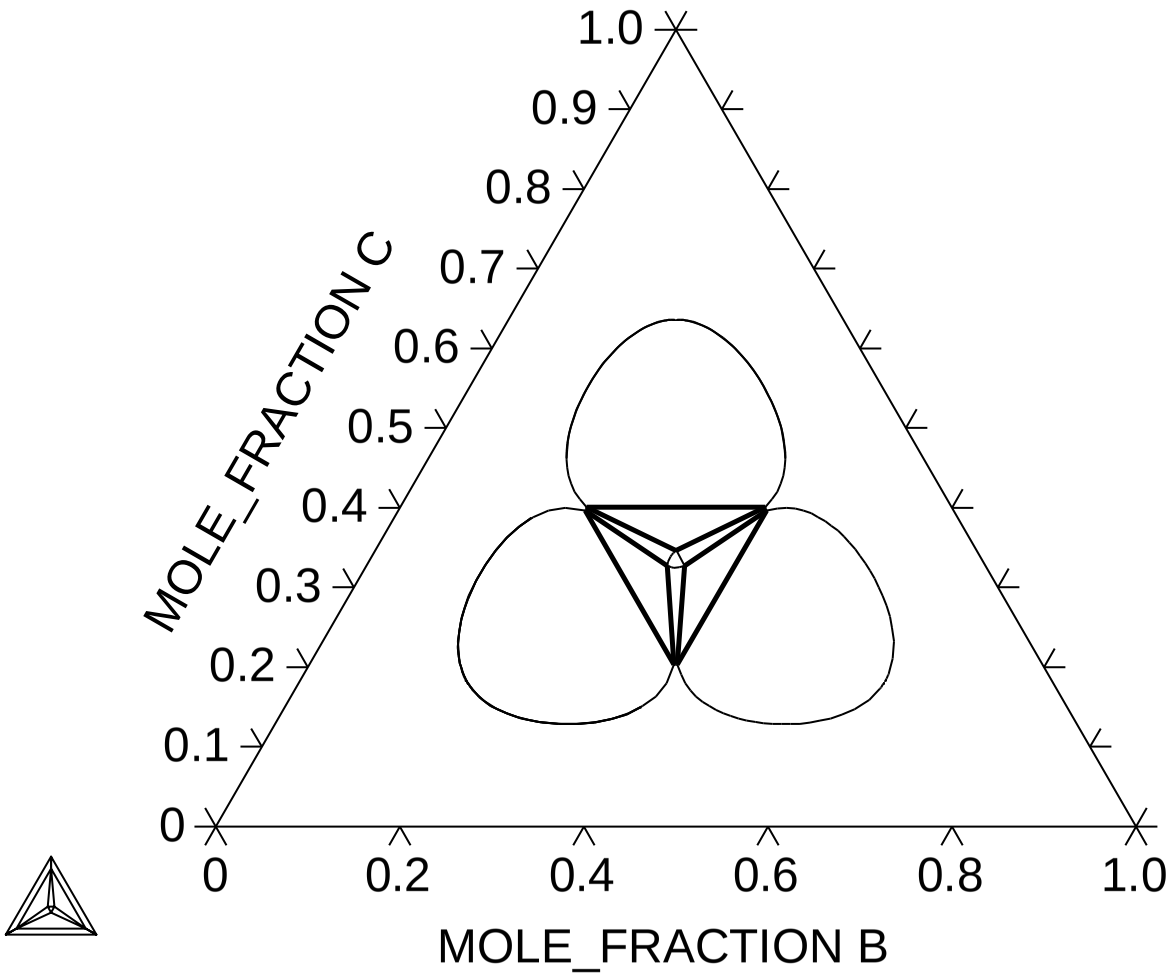
 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,,
POST:
POST:
POST: set-title example 38c
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
 The composition set LIQUID#5 created from the store file
POST:
POST: @?<Hit_return_to_continue>
 CPU time           14  seconds
```

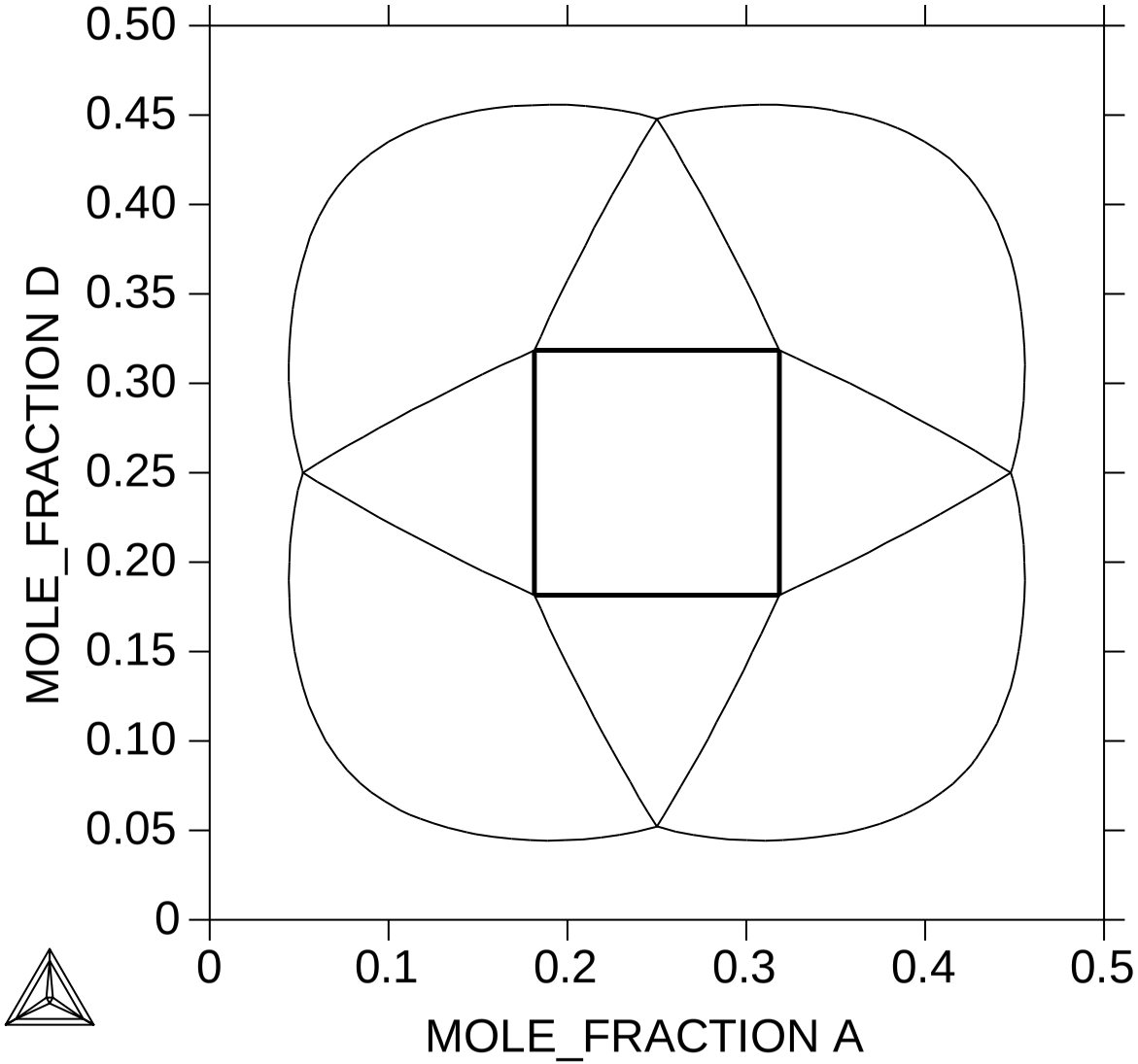
THERMO-CALC (2009.04.15:03.09) :example 38a
DATABASE:User data 2009. 4.15
T=600, P=1E5, N=1;



THERMO-CALC (2009.04.15:03.09) :example 38b
DATABASE:User data 2009. 4.15
T=696, P=1E5, N=1;



THERMO-CALC (2009.04.15:03.09) :example 38c
DATABASE:User data 2009. 4.15
T=170, P=1E5, N=1, X(A)+X(C)=0.5;



39

Calculation of the reversible Carnot cycle of a heat engine

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ The  Calculation of the Reversible Carnot Cycle of Heat Engine
SYS: @@
SYS: @@
SYS: @@ The Reversible Carnot cycles are usually drawn schematically in lectures
SYS: @@ or text books and rarely understood by students. But by making use of
SYS: @@ a thermodynamic software system like Thermo-Calc and realistic data it
SYS: @@ is possible to calculate a reversible Carnot cycle of a heat engine
SYS: @@ and to relate it to different thermodynamic quantities.
SYS: @@ Some particular cases will be calculated and graphicaly presented in this
SYS: @@ example.
SYS: @@
SYS: @@
SYS: @@ One application of the Second Law is to the efficiencies of heat
SYS: @@ engines, pumps and refrigerators.
SYS: @@ Whenever there exists a difference of temperature, work can be
SYS: @@ produced - the principle of heat engines. The Gibbs energy also
SYS: @@ enables us to predict the maximum work that a process may achive.
SYS: @@
SYS: @@
SYS: @@ To illustrate how Thermo-Calc calculates the reversible Carnot cycle we
SYS: @@ will consider one mole of an ideal gas with two ficticious species A
SYS: @@ and A2.
SYS: set-log ex39,,,
SYS:
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
 First version released 1-Jan-78, last update 20-Nov-2007

GES: rei,,,,,
   ... the command in full is REINITIATE
GES: e-e a
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
GES: a-e-d a gas 10,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: e-sp A2 A2
   ... the command in full is ENTER_SPECIES
GES: e-ph gas g 1 A A2; N N
   ... the command in full is ENTER_PHASE
GES: @@ The Gibbs free energy for these specie could be described by
GES: @@ the general formula:  Gm= a +bT + cTlnT + dT2 +...+ RTln(P)
GES: @@
GES: @@ In order to calculate the Carnot cycle one has to give some numerical
GES: @@ values to the a, b, c, etc. constants of the Gm expression.
GES: @@ It is important to understand that the coefficients cannot be
GES: @@ chosen arbirarily, for example c should be negative as the heat capacity
GES: @@ at constant pressure, Cp = - T d2G/dT2 and thus Cp=-c-2dT must always be >0
GES: @@
GES: e-par g(gas,a) 298.15 6960-51*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,,
   ... the command in full is ENTER_PARAMETER
 G(GAS,A;0)-G(GAS,A;0)
GES: e-par g(gas,a2) 298.15 130670-38*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,,
   ... the command in full is ENTER_PARAMETER
 G(GAS,A2;0)- 2 G(GAS,A;0)
GES: l-d,,,,
   ... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH          DATE 2009- 4-15
```

```
 FROM DATABASE: User data 2009. 4.15

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  1 A    GAS                      1.0000E+01  0.0000E+00  0.0000E+00

 SPECIES                                  STOICHIOMETRY
   1 A                                    A
   2 A2                                   A2

 GAS
    CONSTITUENTS: A,A2

      G(GAS,A;0)-G(GAS,A;0) = +6960-51*T-17*T*LN(T)+R*T*LN(1E-05*P)
      G(GAS,A2;0)- 2 G(GAS,A;0) = +130670-38*T-17*T*LN(T)+R*T*LN(1E-05*P)

 SYMBOL        STATUS   VALUE/FUNCTION
   1 R         80000000  8.3145100E+00
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
GES: @?<Hit_return_to_continue>
GES: @@
GES: @@ The Carnot cycle diagram gives the pressure and volume for the
GES: @@ working media of a heat engine that operates between two temperatures
GES: @@ T1 and T2, T1>T2.
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: @@ The Carnot cycle will be calculated for T1=500 K (the temperature
POLY_3: @@ of the hot reservoire) and T2=400 K (the temperature of the cold
POLY_3: @@ reservoire)
POLY_3: ent var t1=500;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent var t2=400;
   ... the command in full is ENTER_SYMBOL
POLY_3: @@
POLY_3: @@ A Carnot cycle consists of four reversible stages:
POLY_3: @@
POLY_3: @@ Stage 1. Isothermal expansion at T1; the entropy change of the system is
POLY_3: @@ Q1/T1, where Q1 is the heat taken from the hot reservoire.
POLY_3: @@
POLY_3: @@
POLY_3: s-c t=t1 p=1e7 n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          137  grid points in           0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  xn
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, P=1E7, N=1
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -5.22193E+04,  Enthalpy  1.54600E+04,  Volume  4.15725E-04

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       1.0000E+00  1.0000E+00 3.5061E-06 -5.2219E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  8.75433E-20
POLY_3: @?<Hit_return_to_continue>
```

```
POLY_3: @@ Set volume to 1 m3
POLY_3: s-c v
   ... the command in full is SET_CONDITION
Value /4.157255E-04/:  1
POLY_3: s-c n
   ... the command in full is SET_CONDITION
Value /1/:  none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, P=1E7, V=1
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  2.40543E+03,  Mass in grams  2.40543E+04
 Total Gibbs energy -1.25610E+08,  Enthalpy  3.71880E+07,  Volume  1.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  8.75433E-20
POLY_3: s-c n
   ... the command in full is SET_CONDITION
Value /2405.433393/:
POLY_3: s-c p
   ... the command in full is SET_CONDITION
Value /10000000/:  none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, N=2405.43, V=1
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  2.40543E+03,  Mass in grams  2.40543E+04
 Total Gibbs energy -1.25610E+08,  Enthalpy  3.71880E+07,  Volume  1.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  8.75433E-20
POLY_3: enter var ha=h;
   ... the command in full is ENTER_SYMBOL
POLY_3: enter var sa=s;
   ... the command in full is ENTER_SYMBOL
POLY_3: s-c s
   ... the command in full is SET_CONDITION
Value /325596.1064/:  sa
POLY_3: s-c v=none
   ... the command in full is SET_CONDITION
```

```
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, N=2405.43, S=SA
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  2.40543E+03,  Mass in grams  2.40543E+04
 Total Gibbs energy -1.25610E+08,  Enthalpy  3.71880E+07,  Volume  1.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  8.75433E-20
POLY_3: @?<Hit_return_to_continue>
POLY_3: show t,p,v,g,n,h,s
   ... the command in full is SHOW_VALUE
 T=500
 P=1E7
 V=1.
 G=-1.2561005E8
 N=2405.4334
 H=3.7188E7
 S=325596.11
POLY_3: @?<Hit_return_to_continue>
POLY_3: ent var ga=g;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent var pa=p;
   ... the command in full is ENTER_SYMBOL
POLY_3: ent var va=v;
   ... the command in full is ENTER_SYMBOL
POLY_3: @@
POLY_3: @@
POLY_3: save tcex39a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: s-c t=500
   ... the command in full is SET_CONDITION
POLY_3: s-c s=204200
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 204000 205000,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          137  grid points in            0  s
    17 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    204200.
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04400E+05 .... OK
 Global test at  2.04650E+05 .... OK
 Global test at  2.04900E+05 .... OK
 Terminating at    205000.
 Calculated    35 equilibria
```

```
 Phase Region from    204200.     for:
     GAS
 Global test at  2.04000E+05 .... OK
 Terminating at    204000.
 Calculated    11 equilibria
 *** Buffer saved on file: tcex39a.POLY3
POLY_3: @@
POLY_3: @@
POLY_3: @@ Stage 2. Adiabatic expansion. No heat leaves the system, so the
POLY_3: @@ change in its entropy is zero. In the course of this expansion the
POLY_3: @@ temperature falls from T1 to T2, the temperature of cold reservoire.
POLY_3: @@
POLY_3: s-c s=205000
   ... the command in full is SET_CONDITION
POLY_3: s-c t=450
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 500,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          137  grid points in           0  s
    13 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    450.000     for:
     GAS
 Global test at  4.70000E+02 .... OK
 Global test at  4.95000E+02 .... OK
 Terminating at    500.000
 Calculated    23 equilibria

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Terminating at    400.000
 Calculated    23 equilibria
 *** Buffer saved on file: tcex39a.POLY3
POLY_3: @@
POLY_3: @@ Stage 3. Isothermal compresion at T2. The heat Q2 is released to the
POLY_3: @@ cold reservoire, so the change in entropy of the system is -Q2/T2.
POLY_3: @@
POLY_3: s-c t=400
   ... the command in full is SET_CONDITION
POLY_3: s-c s=204200
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 204000 205000,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          137  grid points in           0  s
     8 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    204200.
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04400E+05 .... OK
```

```
 Global test at  2.04650E+05 .... OK
 Global test at  2.04900E+05 .... OK
 Terminating at    205000.
 Calculated    35 equilibria

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04000E+05 .... OK
 Terminating at    204000.
 Calculated    11 equilibria
 *** Buffer saved on file: tcex39a.POLY3
POLY_3: @@
POLY_3: @@
POLY_3: @@ Stage 4. Adiabatic compression. No heat enters the system, so the change
POLY_3: @@ in entropy is zero. The temperature rises from T2 to T1.
POLY_3: @@
POLY_3: @@
POLY_3: s-c s=204000
   ... the command in full is SET_CONDITION
POLY_3: s-c t=450
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 500,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          137  grid points in            0  s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    450.000     for:
     GAS
 Global test at  4.70000E+02 .... OK
 Global test at  4.95000E+02 .... OK
 Terminating at    500.000
 Calculated    23 equilibria

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Terminating at    400.000
 Calculated    23 equilibria
 *** Buffer saved on file: tcex39a.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,,,,,,,
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ The efficiency E of an engine which uses a Carnot cycle is:
POST: @@
POST: @@ E=work performed/heat absorbed = W/Q1
```

POST: *@@ If one plots the entropy versus temperature, one can calculate the*
POST: *@@ work performed just by calculating the area of the surface*
POST: *@@ depicted by the two squares and by making the difference between them.*
POST: *@@*
POST: **s-d-a x s**
   ... the command in full is SET_DIAGRAM_AXIS
POST: **s-d-a y t**
   ... the command in full is SET_DIAGRAM_AXIS
POST: **s-s y n 0 600**
   ... the command in full is SET_SCALING_STATUS
POST: **s-s x n 203500 205500**
   ... the command in full is SET_SCALING_STATUS
POST: **set-title example 39b**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@*
POST: *@@*
POST: *@@ The influence of the value of the temperature T1 (the temperature of the*
POST: *@@ hot reservoire) on the efficency of the Carnot cycle is important.*
POST: *@@ Therefor we will make an other calculation for T1=800 K and compare with*
POST: *@@ the one for T1=500 K (example 39a and b). T2=400 K in both cases.*
POST: **ba**
   ... the command in full is BACK
POLY_3: **read,,,**
   ... the command in full is READ_WORKSPACES
POLY_3: **l-c**
   ... the command in full is LIST_CONDITIONS
 T=T1, N=2405.43, S=SA
 DEGREES OF FREEDOM 0
POLY_3: **s-c s=none**
   ... the command in full is SET_CONDITION
POLY_3: **s-c t=800 p=1e7 n=1**
   ... the command in full is SET_CONDITION
POLY_3: **c-e**
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated   137 grid points in   0 s
POLY_3: **l-e**
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VXNS/: **xn**
 Output from POLY-3, equilibrium =   1, label A0 , database: User dat

 Conditions:
 T=800, P=1E7, N=1
 DEGREES OF FREEDOM 0

 Temperature   800.00 K (526.85 C), Pressure 1.000000E+07
 Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
 Total Gibbs energy -9.41189E+04, Enthalpy 2.05600E+04, Volume 6.65161E-04

 Component   Moles   M-Fraction Activity   Potential Ref.stat
 A   1.0000E+00 1.0000E+00 7.1585E-07 -9.4119E+04 SER

 GAS   Status ENTERED   Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00 Mole fractions:
 A 1.00000E+00
 Constitution:
 A   1.00000E+00 A2 1.27812E-15
POLY_3: *@@ Set volume to 1 m3*
POLY_3: **s-c v**
   ... the command in full is SET_CONDITION
Value /6.651608E-04/: **1**
POLY_3: **s-c n**
   ... the command in full is SET_CONDITION
Value /1/: **none**
POLY_3: **c-e**
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid

```
     7 ITS,  CPU TIME USED   0 SECONDS
POLY_3: s-c n
   ... the command in full is SET_CONDITION
Value /1503.395871/:
POLY_3: s-c p
   ... the command in full is SET_CONDITION
Value /10000000/:  none
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          137  grid points in            0  s
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: enter var ha=h;
   ... the command in full is ENTER_SYMBOL
POLY_3: enter var sa=s;
   ... the command in full is ENTER_SYMBOL
POLY_3: s-c s
   ... the command in full is SET_CONDITION
Value /215509.7923/:  sa
POLY_3: s-c v=none
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: show t,p,v,g,n,h,s
   ... the command in full is SHOW_VALUE
 T=800
 P=1E7
 V=1.
 G=-1.4149801E8
 N=1503.3959
 H=3.0909819E7
 S=215509.79
POLY_3: @?<Hit_return_to_continue>
POLY_3: save tcex39b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: s-c s=272000
   ... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 270200 276200,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated          137  grid points in            0  s
    55 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    272000.
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    272000.     for:
     GAS
 Global test at  2.73200E+05 .... OK
 Global test at  2.74700E+05 .... OK
 Global test at  2.76200E+05 .... OK
 Terminating at    276200.
 Calculated    31 equilibria

 Phase Region from    272000.     for:
     GAS
 Global test at  2.70800E+05 .... OK
 Terminating at    270200.
 Calculated    15 equilibria
 *** Buffer saved on file: tcex39b.POLY3
POLY_3: s-c s=276200
   ... the command in full is SET_CONDITION
```

POLY_3: **s-c t=750**
   ... the command in full is SET_CONDITION
POLY_3: **s-a-v 1 t 400 800,,,,**
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: **c-e**
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated   137 grid points in   0 s
    14 ITS, CPU TIME USED   0 SECONDS
POLY_3: **step norm**
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   750.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from   750.000   for:
     GAS
 Terminating at   800.000
 Calculated   8 equilibria

 Phase Region from   750.000   for:
     GAS
 Global test at 6.70000E+02 .... OK
 Global test at 5.70000E+02 .... OK
 Global test at 4.70000E+02 .... OK
 Terminating at   400.000
 Calculated   38 equilibria
 *** Buffer saved on file: tcex39b.POLY3
POLY_3: **s-c t=400**
   ... the command in full is SET_CONDITION
POLY_3: **s-c s=270250**
   ... the command in full is SET_CONDITION
POLY_3: **s-a-v 1 s 270200 276200,,,**
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: **c-e**
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated   137 grid points in   0 s
     9 ITS, CPU TIME USED   0 SECONDS
POLY_3: **step norm**
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   270250.
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from   270250.   for:
     GAS
 Global test at 2.71450E+05 .... OK
 Global test at 2.72950E+05 .... OK
 Global test at 2.74450E+05 .... OK
 Global test at 2.75950E+05 .... OK
 Terminating at   276200.
 Calculated   43 equilibria

 Phase Region from   270250.   for:
     GAS
 Terminating at   270200.
 Calculated   4 equilibria
 *** Buffer saved on file: tcex39b.POLY3
POLY_3: **s-c s=270200**
   ... the command in full is SET_CONDITION
POLY_3: **s-c t=750**
   ... the command in full is SET_CONDITION
POLY_3: **s-a-v 1 t 400 800,,,**
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: **c-e**
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global

```
 Testing POLY result by global minimization procedure
 Calculated          137  grid points in            0  s
    24 ITS,  CPU TIME USED   0 SECONDS
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    750.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    750.000     for:
     GAS
 Terminating at    800.000
 Calculated     8 equilibria

 Phase Region from    750.000     for:
     GAS
 Global test at  6.70000E+02 .... OK
 Global test at  5.70000E+02 .... OK
 Global test at  4.70000E+02 .... OK
 Terminating at    400.000
 Calculated    38 equilibria
 *** Buffer saved on file: tcex39b.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,,,,
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-d-a x s
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 269000 276100
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1000
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 39d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ The efficiency for high value of T1 temperature is almost double compared
POST: @@ with that one for low value of T1 temperature (compare example 39b with
POST: @@ example 39d).
POST: @@
POST: @@ Now we will calculate the Carnot cycle for some real systems. The most
POST: @@ well known engine is the steam engine.
POST: @@
POST: @@ The Carnot cycle for steam engine
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: go d
   ... the command in full is GOTO_MODULE
TDB_TCFE6: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 IONIC_LIQ:Y            L12_FCC                B2_BCC
 B2_VACANCY             HIGH_SIGMA             DICTRA_FCC_A1
```

```
   REJECTED
 REINITIATING GES5 .....
TDB_TCFE6: sw psub
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Pure Substances TDB v1

 VA  DEFINED
TDB_PSUB: def-sp h2o1
   ... the command in full is DEFINE_SPECIES
 H2O1  DEFINED
TDB_PSUB: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:  CONSTITUENTS
 GAS:G       :H2O1:
  > Gaseous Mixture, using the ideal gas model
 H2O_L       :H2O1:
TDB_PSUB: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous species, stoichiometric solids and
      liquids in the Cu-Fe-H-N-O-S system.'
 -OK-
TDB_PSUB: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:  CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 H2O_L                   ENTERED    0.00000000E+00  0.00000000E+00
 GAS                     ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY_3: c-st p h2o_l=sus
   ... the command in full is CHANGE_STATUS
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:  CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 GAS                     ENTERED    0.00000000E+00  0.00000000E+00
 SUSPENDED PHASES:
 H2O_L
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY_3: @@ The Carnot cycle will be calculated for T1=350 K and T2=450 K
POLY_3: @@
POLY_3: s-c t=380 p=1e5 n=100 ac(o)=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated           1  grid points in           0  s
```

```
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VXNS/:  xn
 Output from POLY-3, equilibrium =     1, label A0  , database: PSUB

 Conditions:
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature    380.00 K (   106.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.04643E+07,  Enthalpy -7.96861E+06,  Volume  1.05317E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 2.6556E-22 -1.5697E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY_3: s-c p=none
   ... the command in full is SET_CONDITION
POLY_3: s-c s
   ... the command in full is SET_CONDITION
Value /6567.729208/:  6100
POLY_3: s-c t=350
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated            1  grid points in            0  s
    11 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PSUB

 Conditions:
 T=350, N=100, AC(O)=1, S=6100
 DEGREES OF FREEDOM 0

 Temperature    350.00 K (    76.85 C),  Pressure  3.863618E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.01376E+07,  Enthalpy -8.00259E+06,  Volume  2.51067E-01

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 2.0244E-23 -1.5206E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY_3: @@ step in S with t=350
POLY_3: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex39c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    6100.00     for:
     GAS
 Global test at  6.30000E+03 .... OK
```

```
 Global test at  6.55000E+03 .... OK
 Global test at  6.80000E+03 .... OK
 Terminating at    7000.00
 Calculated    39 equilibria

 Phase Region from    6100.00     for:
     GAS
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file: tcex39c.POLY3
POLY_3:
POLY_3:
POLY_3: read,,,,
   ... the command in full is READ_WORKSPACES
POLY_3: s-c s=6000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated            1  grid points in           0  s
     8 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ step in T with S=6000
POLY_3: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    350.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    350.000     for:
     GAS
 Global test at  3.70000E+02 .... OK
 Global test at  3.95000E+02 .... OK
 Global test at  4.20000E+02 .... OK
 Global test at  4.45000E+02 .... OK
 Terminating at    450.000
 Calculated    43 equilibria
 *** Buffer saved on file: tcex39c.POLY3
POLY_3:
POLY_3: read,,,,
   ... the command in full is READ_WORKSPACES
POLY_3: s-c t=450
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated            1  grid points in           0  s
     9 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Step in S with t=450
POLY_3: @@@@
POLY_3: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    6100.00     for:
     GAS
 Global test at  6.30000E+03 .... OK
 Global test at  6.55000E+03 .... OK
 Global test at  6.80000E+03 .... OK
 Terminating at    7000.00
 Calculated    39 equilibria

 Phase Region from    6100.00     for:
```

```
     GAS
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file: tcex39c.POLY3
POLY_3:
POLY_3: s-c s=7000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated            1  grid points in           0  s
    41 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Step in T with S=7000
POLY_3: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Global test at  3.80000E+02 .... OK
 Global test at  3.55000E+02 .... OK
 Terminating at    350.000
 Calculated    43 equilibria
 *** Buffer saved on file: tcex39c.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-p-f ##1,,,,,,,,
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39e
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39f
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ It is a bit difficult to distinguish from the calculated diagram,
POST: @@ example 39e, where the adiabatic expansion and compresion start.
POST: @@ Therefore it is good to plot on the same diagram also the temperature.
POST: @@
POST: s-d-a z t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab none
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39g
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
```

```
POST: @?<Hit_return_to_continue>
POST: @@
POST: @@ With Thermo-Calc one may also calculate the Carnot cycle  for real systems
POST: @@ and also include phase transformations.
POST: @@
POST: @@ Trying a Carnot cycle for water - it shows the case with H2O_liquid
POST: @@ to gas phase transformation. In the calculations the volum of the liquid
POST: @@ water was ignored.
POST: @@
POST: ba
   ... the command in full is BACK
POLY_3: go d
   ... the command in full is GOTO_MODULE
TDB_PSUB: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
TDB_PSUB: sw psub
   ... the command in full is SWITCH_DATABASE
TDB_PSUB: def-sp h2o1
   ... the command in full is DEFINE_SPECIES
 H2O1  DEFINED
TDB_PSUB: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/:  CONSTITUENTS
 GAS:G       :H2O1:
  > Gaseous Mixture, using the ideal gas model
 H2O_L       :H2O1:
TDB_PSUB: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous species, stoichiometric solids and
      liquids in the Cu-Fe-H-N-O-S system.'
 -OK-
TDB_PSUB: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:  CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 H2O_L                   ENTERED    0.00000000E+00  0.00000000E+00
 GAS                     ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY_3: c-st p h2o_l=e 0
   ... the command in full is CHANGE_STATUS
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:  CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 H2O_L                   ENTERED    0.00000000E+00  0.00000000E+00
 GAS                     ENTERED    0.00000000E+00  0.00000000E+00
```

```
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY_3: s-c t=380 p=1e5 n=100 ac(o)=1
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated            2  grid points in            0  s
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VXNS/:  xn
 Output from POLY-3, equilibrium =     1, label A0  , database: PSUB

 Conditions:
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature    380.00 K (   106.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.04643E+07,  Enthalpy -7.96861E+06,  Volume  1.05317E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 2.6556E-22 -1.5697E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY_3: s-c p=none
   ... the command in full is SET_CONDITION
POLY_3: s-c s
   ... the command in full is SET_CONDITION
Value /6567.729208/:  6100
POLY_3: s-c t=350
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated            2  grid points in            0  s
    36 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PSUB

 Conditions:
 T=350, N=100, AC(O)=1, S=6100
 DEGREES OF FREEDOM 0

 Temperature    350.00 K (    76.85 C),  Pressure  4.130267E+04
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.03545E+07,  Enthalpy -8.21947E+06,  Volume  1.98337E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 6.6188E-24 -1.5532E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 8.4450E+01, Mass 5.0711E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00

 H2O_L                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.5550E+01, Mass 9.3379E+01, Volume fraction 0.0000E+00  Mole fractions:
```

```
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY_3: @@ step in S with t=350
POLY_3: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex39d y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    6100.00     for:
     GAS
     H2O_L
 Global test at  6.30000E+03 .... OK
 Global test at  6.55000E+03 .... OK
 Global check of removing phase at  6.71967E+03
 Calculated    27 equilibria

 Phase Region from    6719.67     for:
     GAS
 Global test at  6.90000E+03 .... OK
 Terminating at    7000.00
 Calculated    15 equilibria

 Phase Region from    6100.00     for:
     GAS
     H2O_L
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file: tcex39d.POLY3
POLY_3:
POLY_3: read,,,,
   ... the command in full is READ_WORKSPACES
POLY_3: s-c s=6000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated            2  grid points in            0  s
     6 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ step in T with S=6000
POLY_3: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    350.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    350.000     for:
     GAS
     H2O_L
 Global test at  3.70000E+02 .... OK
 Global test at  3.95000E+02 .... OK
 Global test at  4.20000E+02 .... OK
 Global test at  4.45000E+02 .... OK
 Terminating at    450.000
 Calculated    43 equilibria
 *** Buffer saved on file: tcex39d.POLY3
POLY_3:
POLY_3: read,,,,
   ... the command in full is READ_WORKSPACES
POLY_3: s-c t=450
   ... the command in full is SET_CONDITION
POLY_3: c-e
```

```
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated           2  grid points in           0  s
    12 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Step in S with t=450
POLY_3: @@
POLY_3: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    6100.00     for:
     GAS
     H2O_L
 Global check of removing phase at  6.16203E+03
 Calculated     5 equilibria

 Phase Region from    6162.03     for:
     GAS
 Global test at  6.35000E+03 .... OK
 Global test at  6.60000E+03 .... OK
 Global test at  6.85000E+03 .... OK
 Terminating at    7000.00
 Calculated    37 equilibria

 Phase Region from    6100.00     for:
     GAS
     H2O_L
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file: tcex39d.POLY3
POLY_3:
POLY_3: s-c s=7000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated           2  grid points in           0  s
    40 ITS,  CPU TIME USED   0 SECONDS
POLY_3: @@ Step in T with S=7000
POLY_3: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
 Global calculation of initial equilibrium . impossible due to conditions.
 POLY has calculated initial equilibrium
 Global test of initial equilibrium

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Global test at  3.80000E+02 .... OK
 Global test at  3.55000E+02 .... OK
 Terminating at    350.000
 Calculated    43 equilibria
 *** Buffer saved on file: tcex39d.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

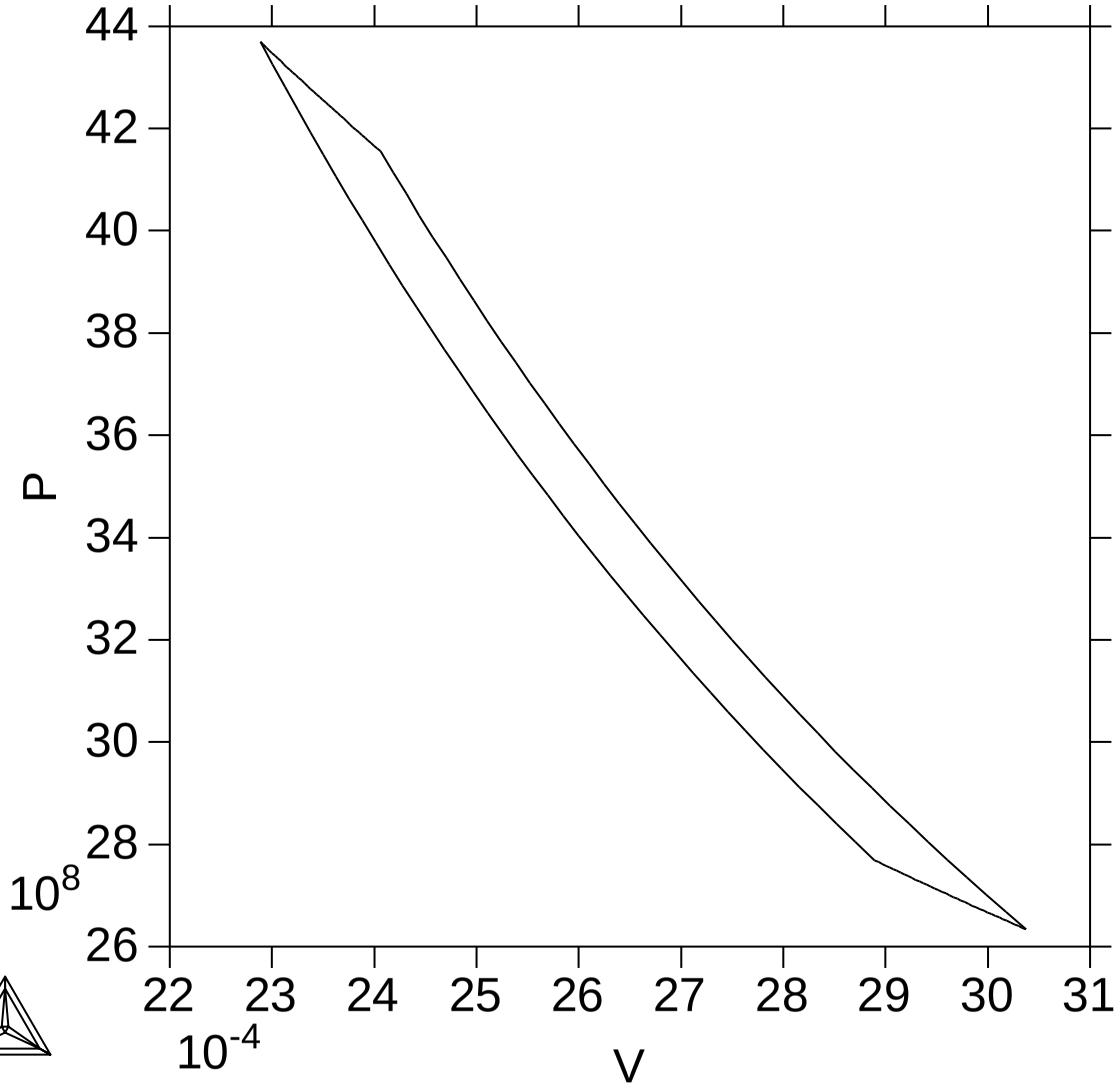
 Setting automatic diagram axis

POST: @@ The cycle shows the constant pressure at phase transformation.
POST: s-p-f ##1,,,,,,,,,
```

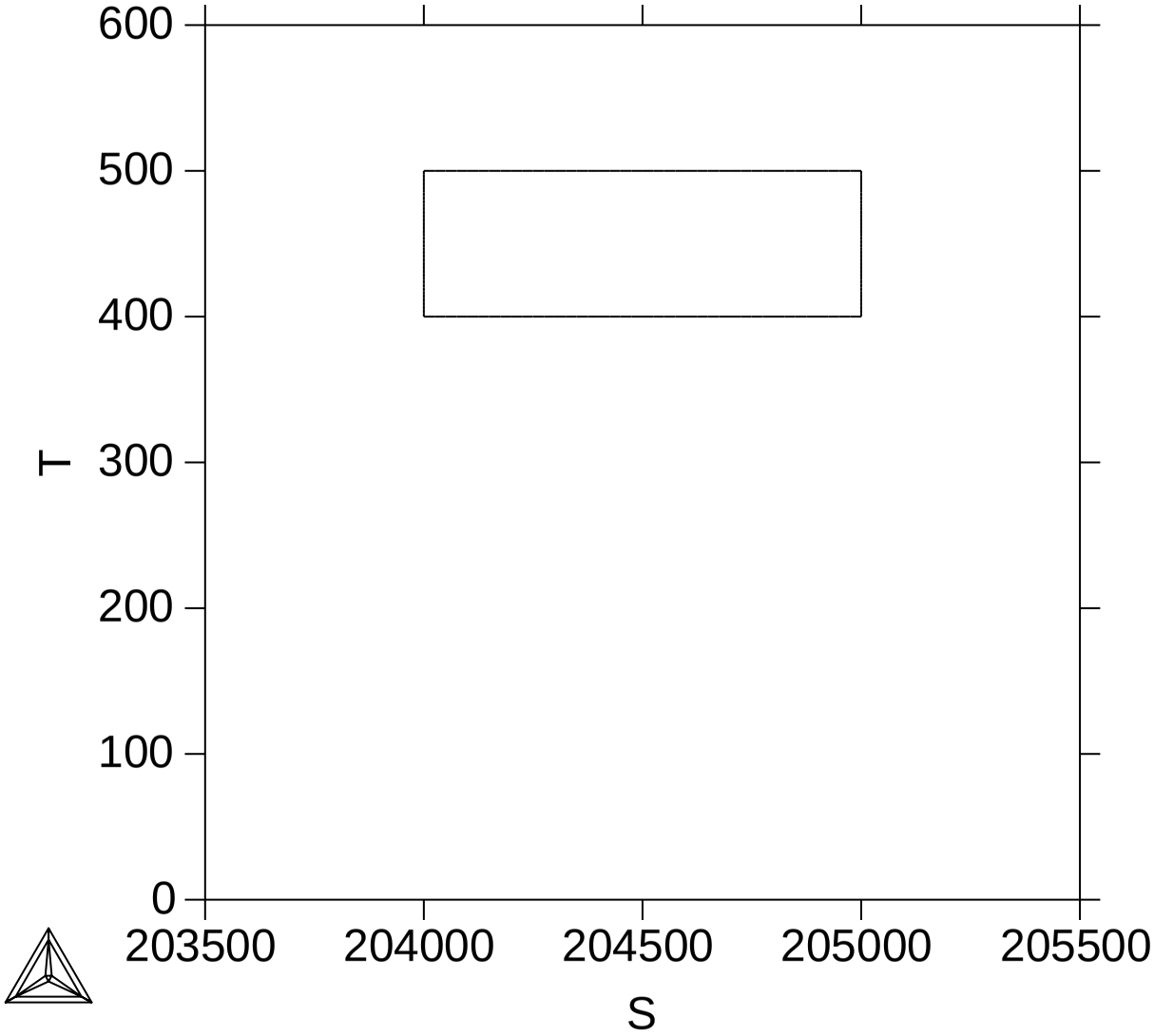
POST:
POST: *@@ To get a better understanding of this process it is now possible to plot*
POST: *@@ the cycle using any set of thermodynamic state variables.*
POST: *@@ Thus, from the pressure-volume-temperature diagram, example 39g, it is*
POST: *@@ possible to see the temperature variation on the two adiabatical stages*
POST: *@@ of the Carnot cycle.*
POST: *@@ The cycle shows the constant pressure at phase transformation.*
POST: **s-d-a x v**
... the command in full is SET_DIAGRAM_AXIS
POST: **s-d-a y p**
... the command in full is SET_DIAGRAM_AXIS
POST: **set-title example 39h**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **s-a-ty y log**
... the command in full is SET_AXIS_TYPE
POST: **s-lab b**
... the command in full is SET_LABEL_CURVE_OPTION
POST: **s-tit example 39i**
... the command in full is SET_TITLE
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **s-d-a z t**
... the command in full is SET_DIAGRAM_AXIS
POST: **s-lab none**
... the command in full is SET_LABEL_CURVE_OPTION
POST: **set-title example 39j**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ Also interesting seems to plot the amount of phases versus volume. One*
POST: *@@ could get information about both the kind and amount of phases which*
POST: *@@ fill up a certain volume.*
POST: **s-d-a z none**
... the command in full is SET_DIAGRAM_AXIS
POST: **s-d-a y np(*),,,**
... the command in full is SET_DIAGRAM_AXIS
POST: **s-a-ty y,,,**
... the command in full is SET_AXIS_TYPE
POST: **s-lab b**
... the command in full is SET_LABEL_CURVE_OPTION
POST: **set-title example 39k**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ Next diagram shows the amount of phases versus pressure. It gives important*
POST: *@@ information on the phase transformation pressure and on the ratio*
POST: *@@ between the two phases in equilibrium at a certain pressure.*
POST: *@@*
POST: **s-d-a x p**
... the command in full is SET_DIAGRAM_AXIS
POST: **set-title example 39l**
POST: **plot**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: *@@ By ploting the amount of phases versus temperature, example 39k, it is*
POST: *@@ possible to know the phase transformation temperature and also the ratio*
POST: *@@ between the two phases in equilibrium at a certain temperature.*
POST: *@@*
POST: **s-d-a x t**
... the command in full is SET_DIAGRAM_AXIS
POST: **set-title example 39m**

POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: ***@@ The enthalpy and Gibbs energy for the Carnot cycle could also be***
POST: ***@@ ploted using the same calculation but a different set for diagram axis.***
POST: ***@@ Note the important drop of the enthalpy at the phase transformation***
POST: ***@@ point, example 39l.***
POST: **s-lab none**
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: **s-d-a x v**
   ... the command in full is SET_DIAGRAM_AXIS
POST: **s-d-a y h**
   ... the command in full is SET_DIAGRAM_AXIS
POST: **s-d-a z t**
   ... the command in full is SET_DIAGRAM_AXIS
POST: **set-title example 39n**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **s-d-a x v**
   ... the command in full is SET_DIAGRAM_AXIS
POST: **s-d-a y g**
   ... the command in full is SET_DIAGRAM_AXIS
POST: **set-title example 39o**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
 CPU time   1 seconds

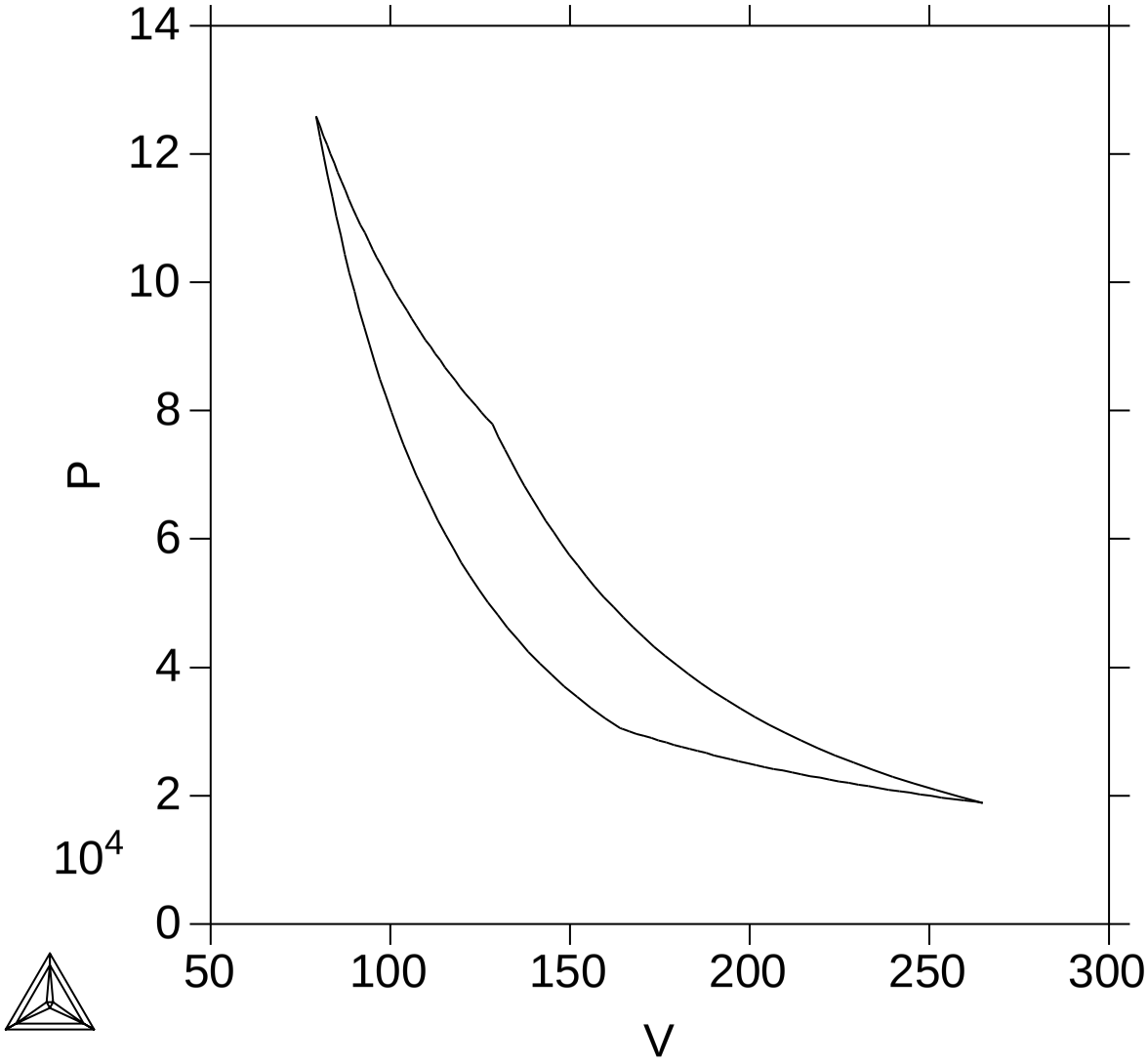
THERMO-CALC (2009.04.15:03.09) :example 39a
DATABASE:User data 2009. 4.15
N=2405.43, S=2.04E5;



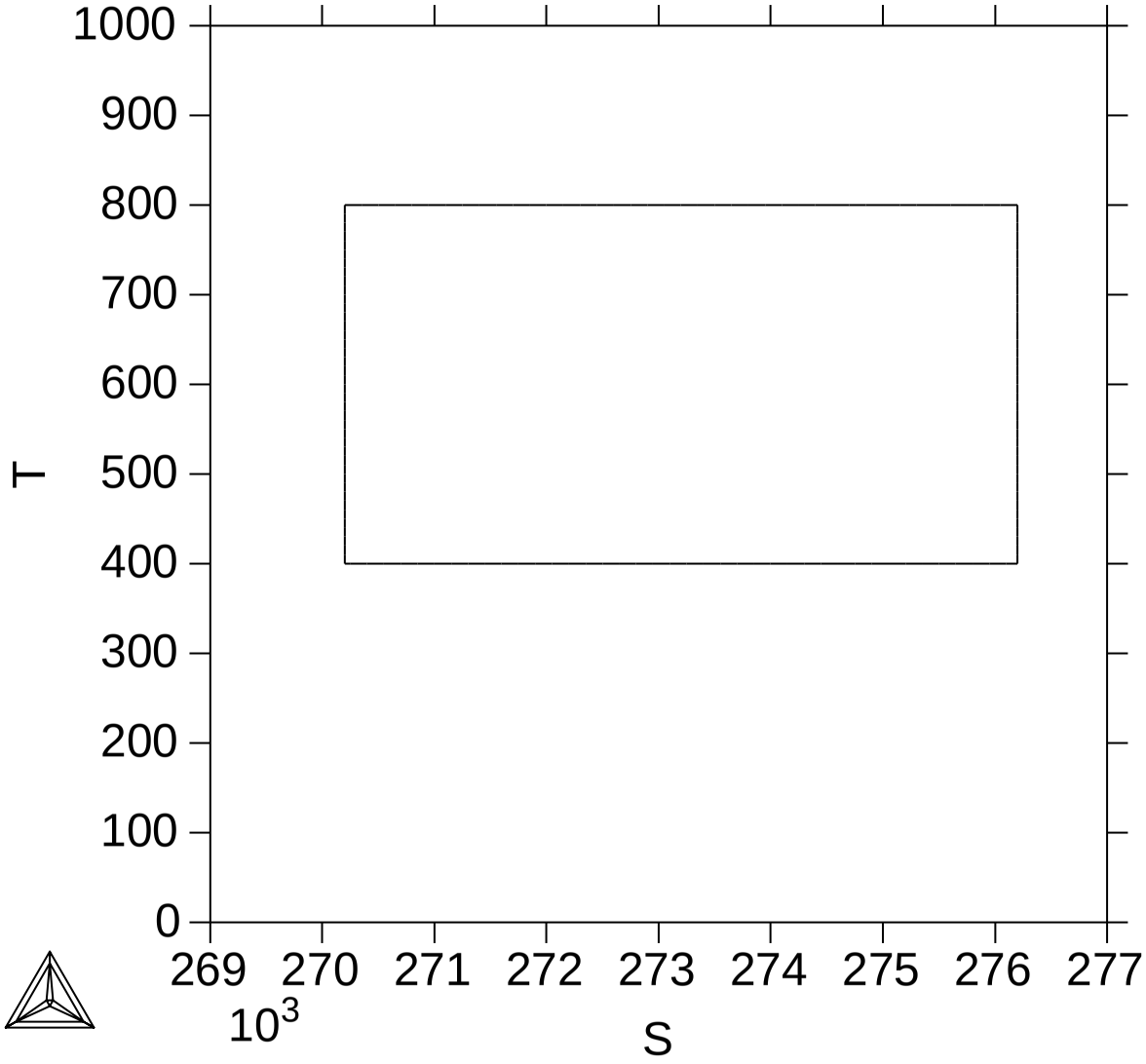
THERMO-CALC (2009.04.15:03.09) :example 39b
DATABASE:User data 2009. 4.15
N=2405.43, S=2.04E5;



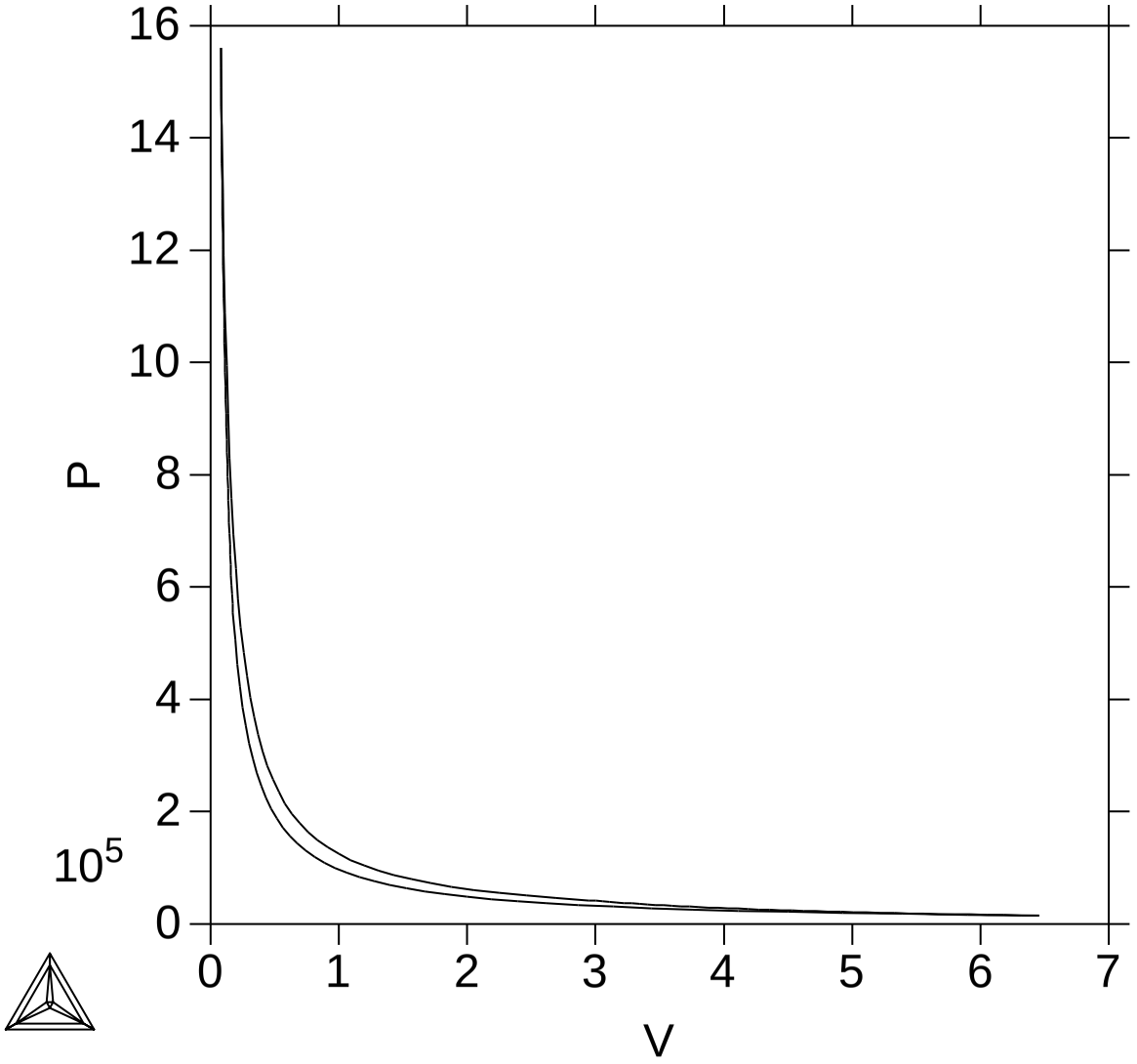
THERMO-CALC (2009.04.15:03.09) :example 39c
DATABASE:User data 2009. 4.15
N=1503.4, S=2.702E5;



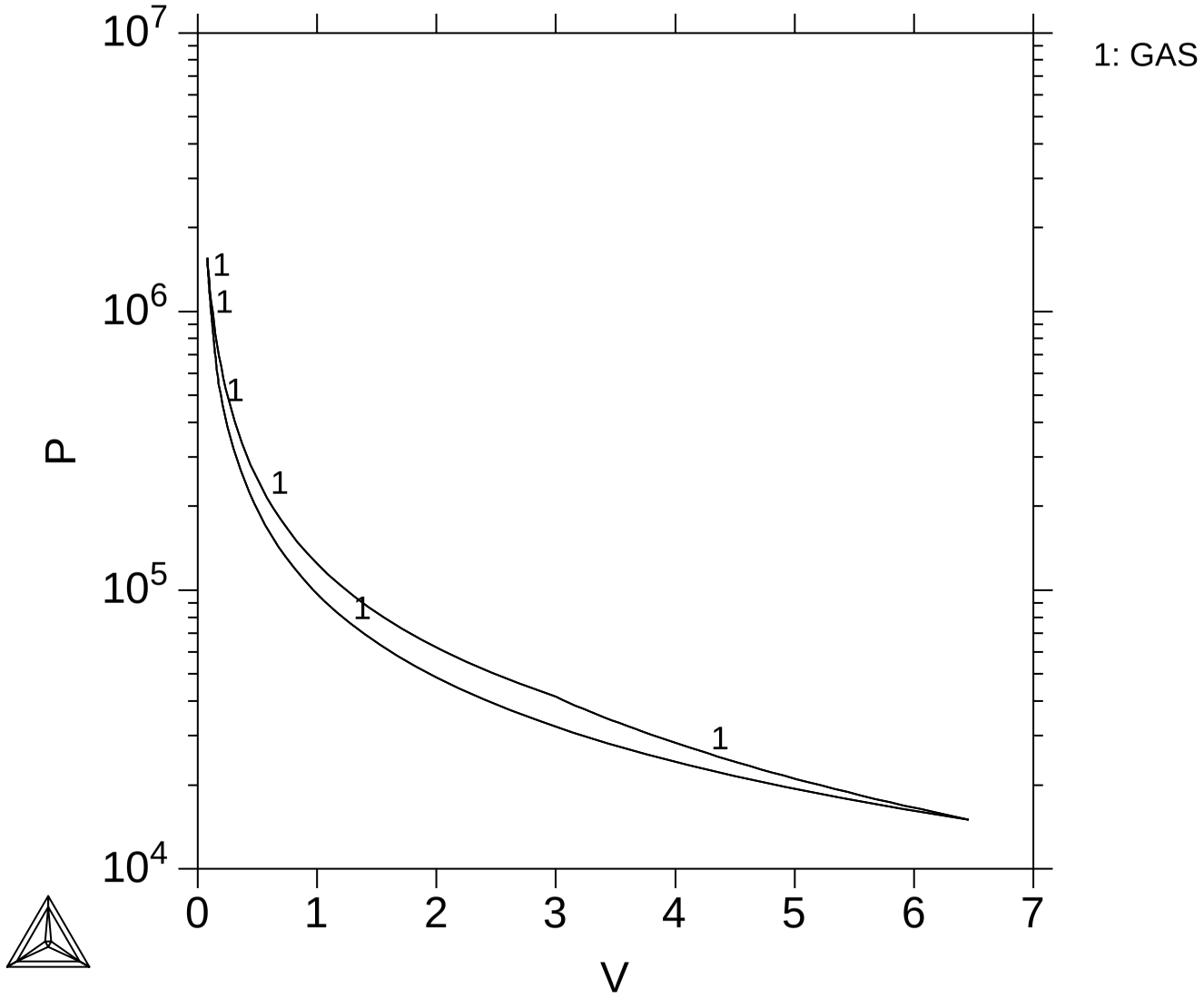
THERMO-CALC (2009.04.15:03.09) :example 39d
DATABASE:User data 2009. 4.15
N=1503.4, S=2.702E5;



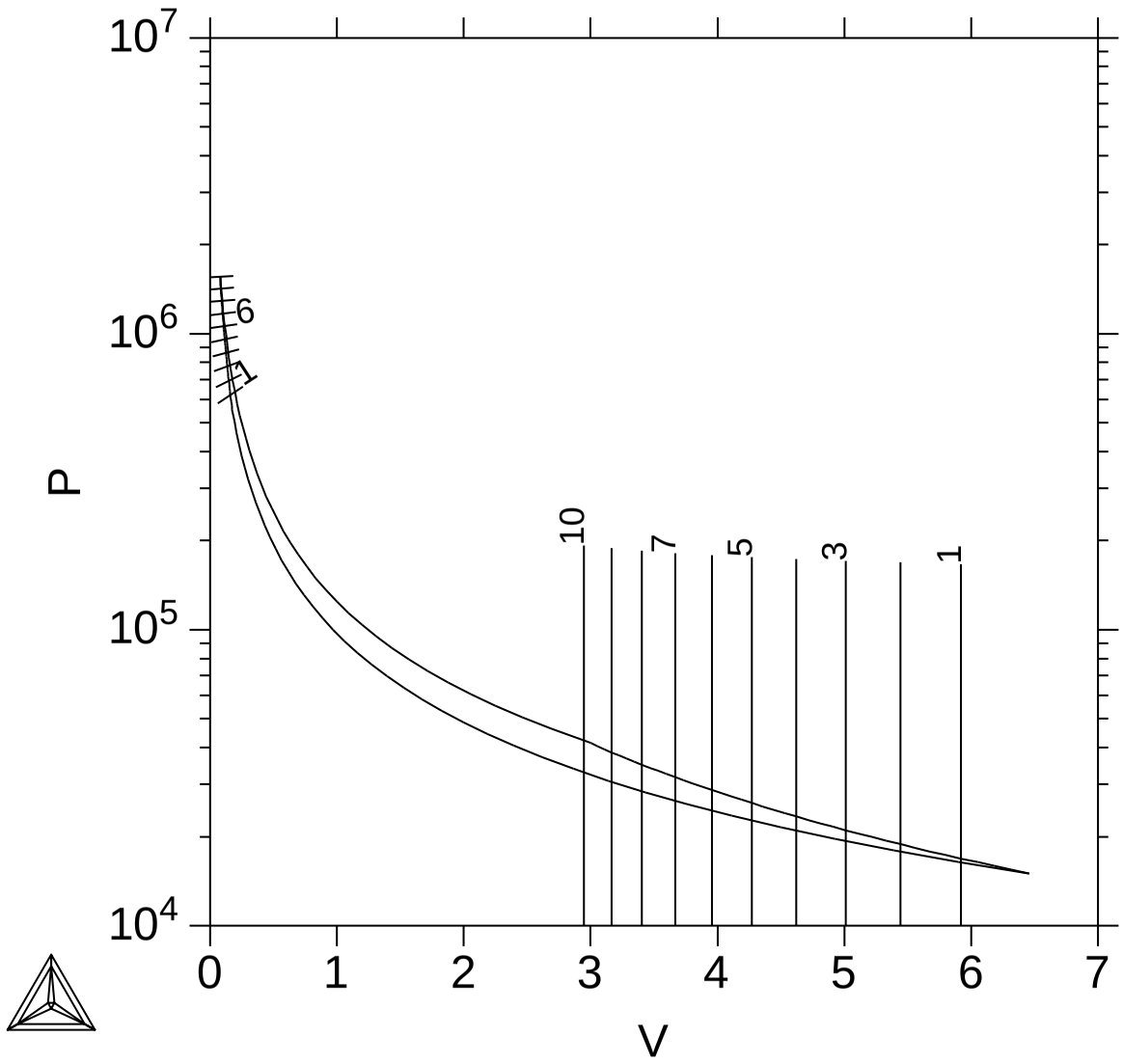
THERMO-CALC (2009.04.15:03.09) :example 39e
DATABASE:PSUB
N=100, AC(O)=1, S=7000.;



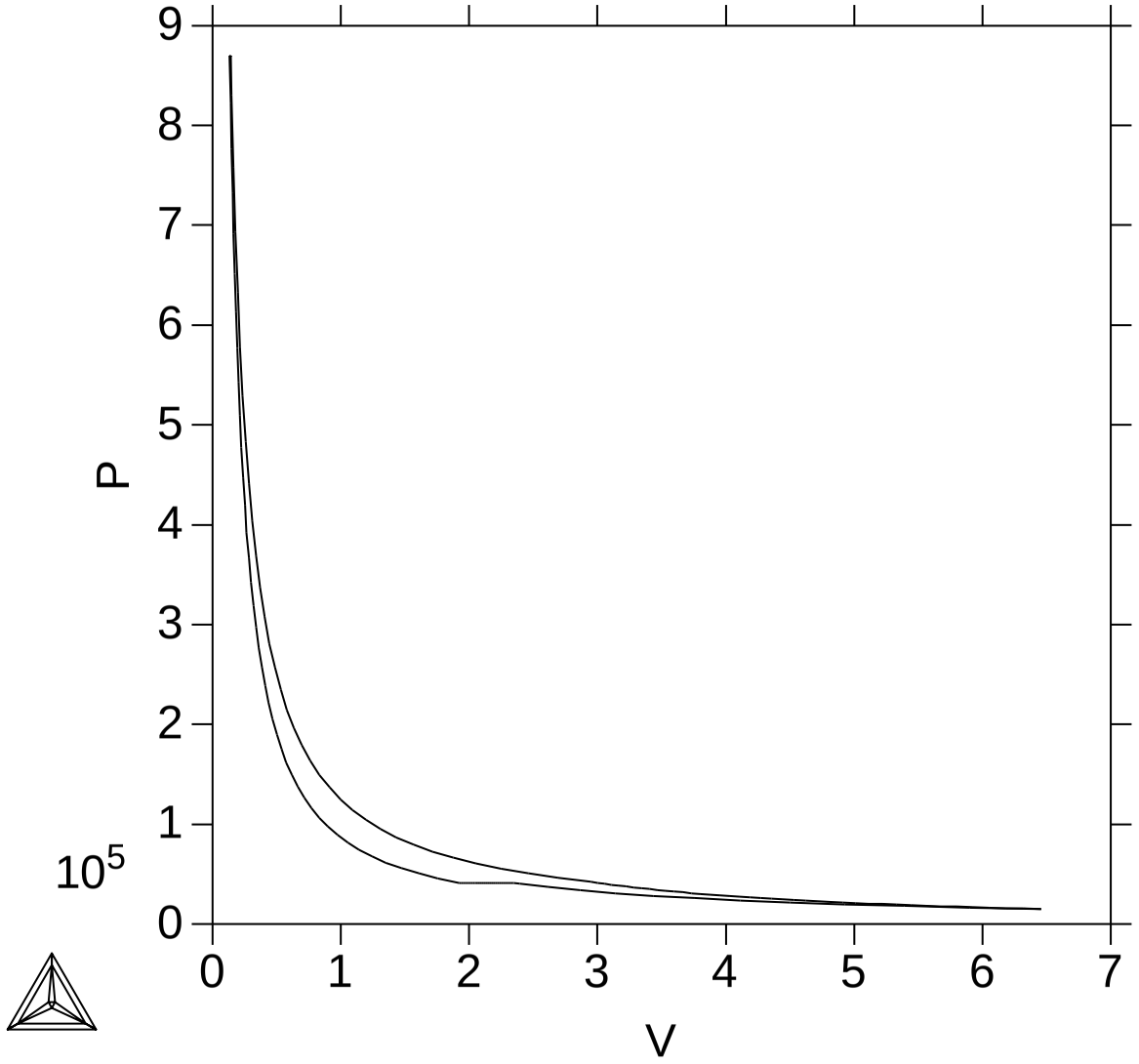
THERMO-CALC (2009.04.15:03.09) :example 39f
DATABASE:PSUB
N=100, AC(O)=1, S=7000.;



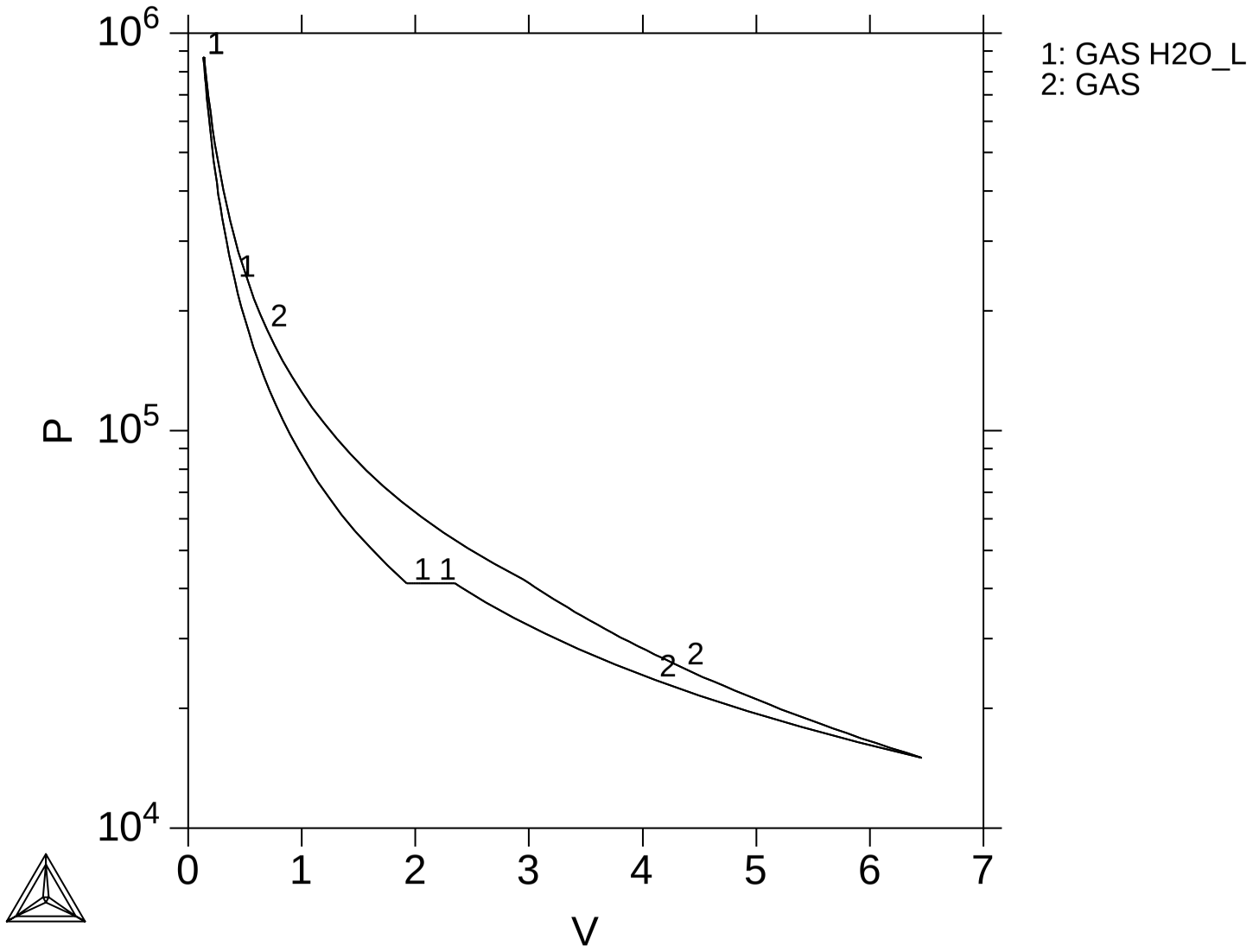
THERMO-CALC (2009.04.15:03.09) :example 39g
DATABASE:PSUB



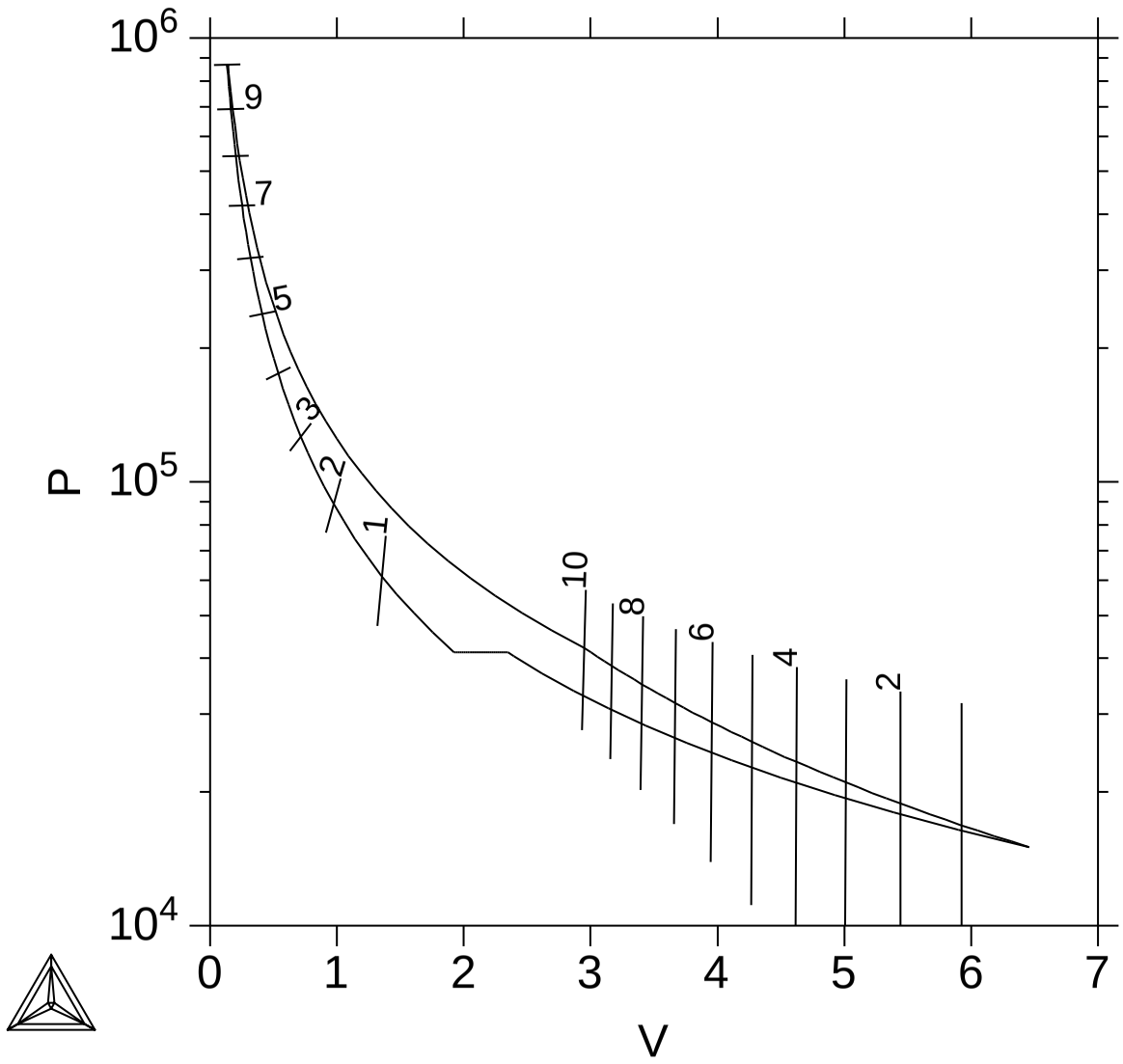
THERMO-CALC (2009.04.15:03.09) :example 39h
DATABASE:PSUB
N=100, AC(O)=1, S=7000.;



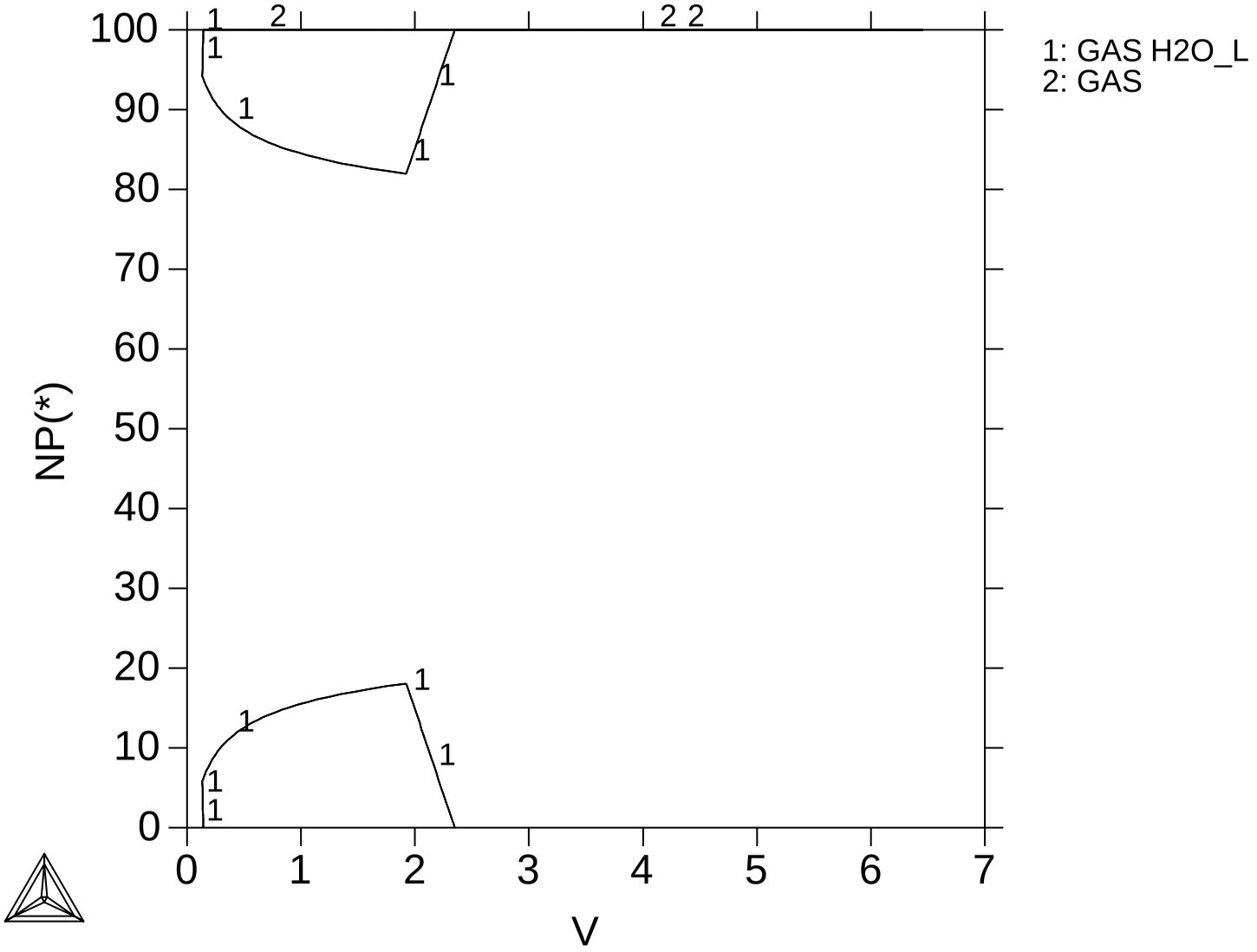
THERMO-CALC (2009.04.15:03.09) :example 39i
DATABASE:PSUB
N=100, AC(O)=1, S=7000.;



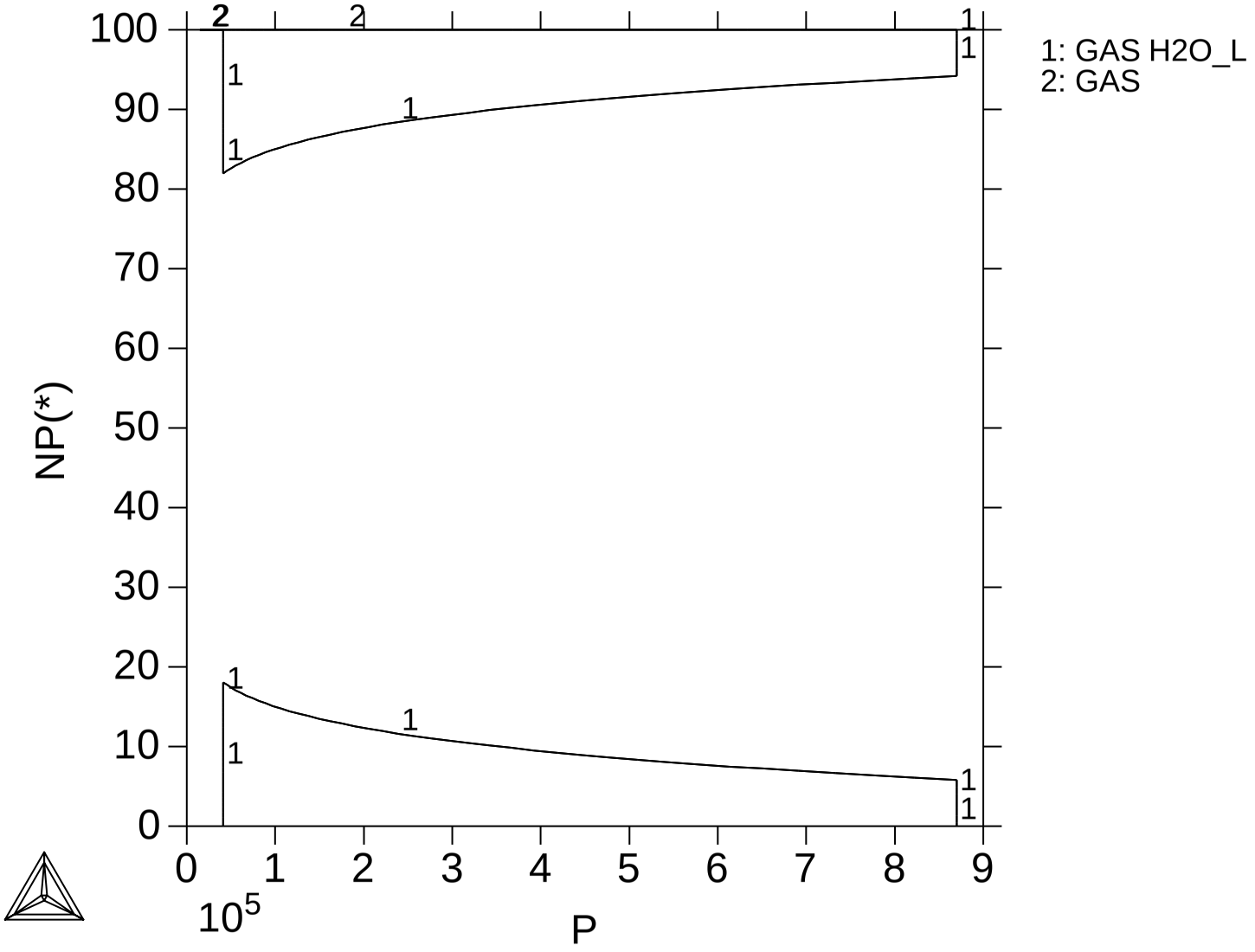
THERMO-CALC (2009.04.15:03.09) :example 39j
DATABASE:PSUB



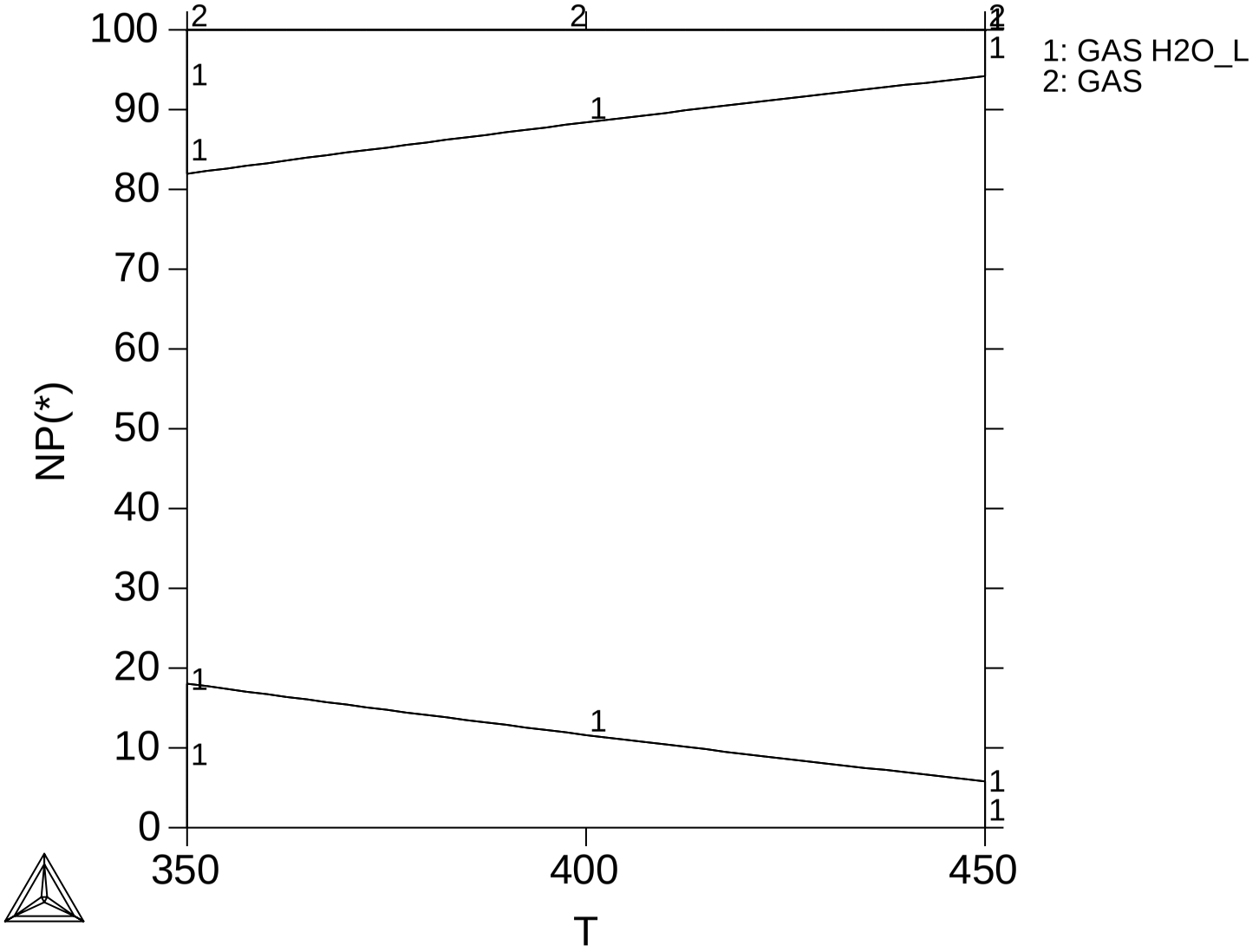
THERMO-CALC (2009.04.15:03.09) :example 39k
DATABASE:PSUB
N=100, AC(O)=1, S=7000.;

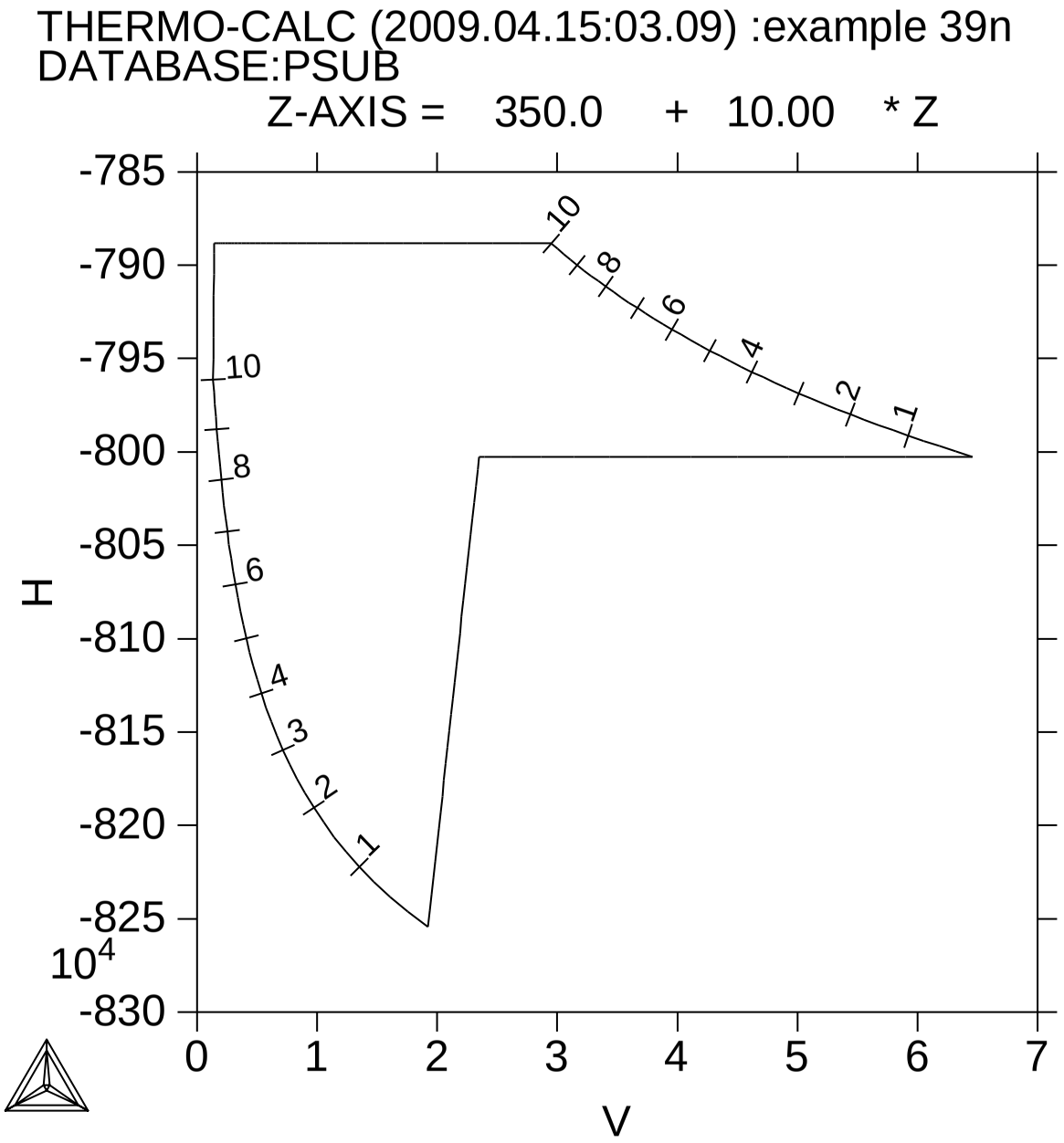


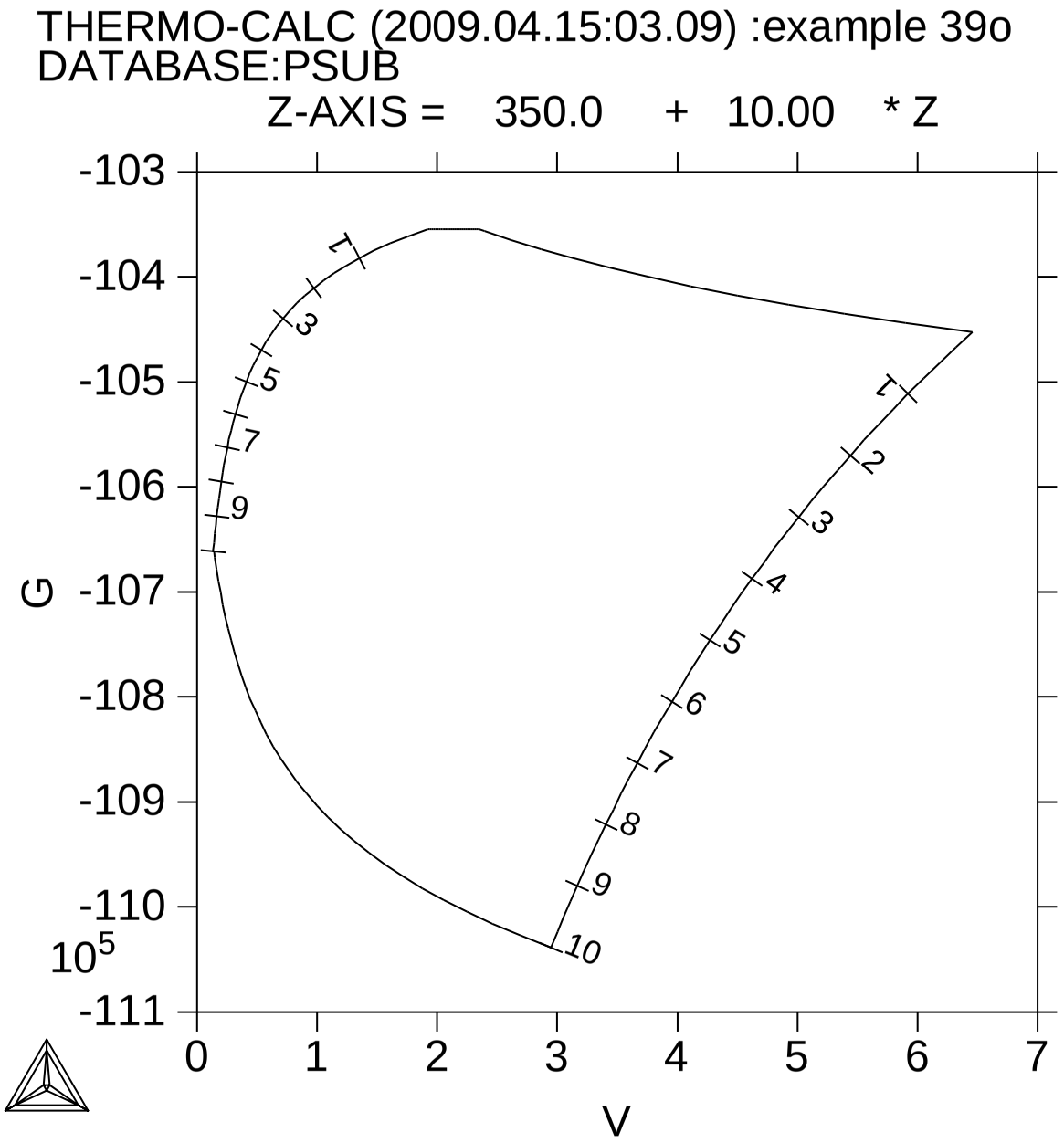
THERMO-CALC (2009.04.15:03.09) :example 39l
DATABASE:PSUB
N=100, AC(O)=1, S=7000.;



THERMO-CALC (2009.04.15:03.09) :example 39m
DATABASE:PSUB
N=100, AC(O)=1, S=7000.;




THERMO-CALC (2009.04.15:03.09) :example 39n
DATABASE:PSUB
Z-AXIS = 350.0 + 10.00 * Z
-785
-790
-795
-800
-805
-810
-815
-820
-825
-830
H
10^4
0
1
2
3
4
5
6
7
V
10
8
6
4
2
1
10
8
6
4
3
2
1


THERMO-CALC (2009.04.15:03.09) :example 39o
DATABASE:PSUB
Z-AXIS = 350.0 + 10.00 * Z
-103
-104
-105
-106
-107
-108
-109
-110
-111
G
10^5
0
1
2
3
4
5
6
7
V
1
3
5
7
9
1
2
3
4
5
6
7
8
9
10

40

POURBAIX module

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: go sys
SYS: set-echo
SYS:
SYS:Heading:SYS:
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS:
SYS:SYS:SYS:SYS:SYS:SYS:
SYS:SYS:SYS:   ... the command in full is GOTO_MODULE

                WELCOME TO THE POURBAIX MODULE
                !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
          for Quick Calculations of Pourbaix Diagrams
          ==========================================

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                    Thermo-Calc Software AB
                   Stockholm Technology Park
                  SE-113 47 Stockholm, Sweden

                   (Version 6.0,  Sep. 2008)

Need any instruction on the POURBAIX module? /N/:
   IMPORTANT NOTES for Calculating a POURBAIX Diagram:
   -----------------------------------------------------------
    1) The so-called Pourbaix diagram is actually a calculated
         equilibrium phase diagram mapped and plotted with the
         independently-varied electropotential (Eh, as defined
         with regard to the standard hydrogen electrode as its
         reference) and acidity (pH), that represents all the
         equilibrated phase boundaries among aqueous solution,
         gaseous mixture, and various primary and secondary
         solids (modelled as either complex solution or simple
         stoichiometric phases) in a certain multicomponent
         heterogeneous interaction system, under a defined T-P
         condition and a specific initial bulk composition
         (which is, by default, always set as 1 kg of water
         dissolving a specified amount of metals/alloys and
         other acids/alkalines/salts).
    2) One must have at least a database containing an AQUEOUS
         solution phase (with thermodynamic data for water and
         various aqueous solutes), that shall be selected from
         TCAQ2 (PAQ2) or AQS2 (PAQS2) [which use the SIT Model
         or Complete Revised HKF Model, respectively] within
         the Thermo-Calc (TCC/TCW) package, or be chosen from
         an appropriate USER-specified database (being in the
         Thermo-Calc TDB format).
    3) Due to the restrictions of aqueous solution model used
         within Thermo-Calc, such a database must be designed
         in the same format as in the default TCAQ2 (PAQ2) or
         AQS2 (PAQS2) for AQUEOUS solution phase; among others,
         one should keep in mind the following regulations:
         * The ELECTRON is defined as an special element (ZE)
           and as the only constituent in its reference phase
           REFERENCE_ELECTRODE (for determining the electro-
           potential that is defined as Eh with the standard
           hydrogen electrode as the reference), but it is
           not defined as an aqueous species;
         * The vacancy (VA) is unnecessary for AQUEOUS solution
           phase and it should be avoided in the definition of
           phase-constituents in the AQUEOUS phase;
         * The AQUEOUS solution phase should always be defined
           as a constitutional solution phase, implying that
           all the aqueous solution species must be included
           in a single site, rather than in two or multiple
           sublattices.
    4) Beside the AQUEOUS solution phase, there shall exist a
         GAS mixture phase containing at least H2O1, O2 and H2;
```

```
          and for multicomponent systems, normally there shall
          also contain some solid (stoichiometric or solution)
          phases. Of course, if desired, you could also choose
          to calculate and generate a Pourbaix diagram without
          considering the GAS mixture phase entirely; however,
          such a plot is not really a complete Pourbaix diagram,
          due to the fact that thermodynamically-stable phase
          boundaries between the AQUEOUS solution phase and GAS
          mixture phase will then not be calculated at all
    5) All thermodynamic data for calculation of a Pourbaix
          diagram should be retrieved from one single database
          which consists of aqueous, gaseous (& solid) phases,
          or from multiple databases which respectively contain
          various phases. All of such suitable databases can be
          the default ones (i.e., in the Single-Database case,
          the PAQ2 or PAQS2; and in the Multiple-Database case,
          the TCAQ2 or AQS2 as the primarily-switched one, plus
          SSUB as the first appended one and SSOL as the second
          appended one if necessary). Of course, you could also
          choose to append required data from other appropriate
          databases (such as TCMP, SLAG, TCFE, TTNi, TTAl, TTMg,
          etc.) for GAS mixture phase and for varous solution
          and stoichiometric phases. Furthermore, an experienced
          user can also utilize his/her USER-specified databases
          in various cases.
    6) The current advanced POURBAIX-Module has been designed
          and developed in an efficient and effective way that
          it only requires the user to just answer some simple
          and necessary questions, rather than to go through
          basic modules (i.e., TDB, GES5, POLY3 and POST) and
          type the ordinary command-lines. Beside the default
          plotted Pourbaix diagram, it also allows the user to
          easily and quickly plot many different properties of
          the system, stable phases and aqueous species, varied
          along the calculated phase boundaries for the same
          defined heterogeneous interaction system. Moreover,
          it permits the user to directly change some plotting
          settings and munipulate all kinds of plotted diagrams.
    7) The current advanced POURBAIX-Module has been extended
          so that it is additionally able to directly perform a
          normal STEPPING calculation (varied with a specified
          independent variable) and to easily generate various
          types of property diagrams, for the same heterogeneous
          interaction system that has been defined in a previous
          POURBAIX or TDB-GES5-PLOY3-POST calculation.
   ------------------------------------------------------------

Enforce a PAUSE after plotting when running a MACRO? /N/:
    Whenever running a TCC MACRO (TCM) file, you may prefer to
    have a PAUSE after a specific diagram has been plotted on
    the SCREEN, for the multiple purposes of efficiently and
    easily manipulating the plotted diagram directly on the
    Thermo-Calc Graph window, such as:
      * Printing it (in EMF or PS graphical format)
          through connected printer(s);
      * Saving it as an EMF graphical file;
      * Dumping it as a PNG or BMP graphical file;
      * Setting background colour for the current diagram
          and for all the sequential plots;
      * Setting default font for all the sequential plots;
      * Changing plotting Layers for all the sequential plots.

    If no PAUSE is enforced, the POURBAIX Module will be going
    through all the sequential command-lines (answers) in the
    same POURBAIX session or till the SET_INTERACTIVE_MODE line
    in the MACRO file has been reached.

    ------------------------------------------------------------
    ** By Y(y), a PAUSE is always enforced after each diagram;
    ** By N(n), no PAUSE will be enforced at any point at all.
    ------------------------------------------------------------
    Please then press <RETURN> at the PAUSE for continuation!

Enforce a PAUSE after plotting when running a MACRO? /N/:
```

```
    ----------------------------------------------------------
   |                                                          |
   |  1. Start a completely new POURBAIX diagram calculation  |
   |  2. Open an old file & plot other property diagrams      |
   |  3. Open an old file & make another POURBAIX calculation |
   |  4. Open an old file & make another STEPPING calculation |
   |                                                          |
    ----------------------------------------------------------

Select option /1/:
   One of the four options (1/2/3/4) should be entered here:

    1 -- Make a completely new POURBAIX diagram calculation
           and automatically plot a pH-Eh diagram.
              i.e., define a new chemical system;
                    specify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.

    2 -- Open an existing POLY3 file created by POURBAIX Module
            (from a previous POURBAIX calculation Option 1 or 3
              or  a previous STEPPING calculation Option 4),
           and just selectively plot other property diagrams.
              i.e., open the old GES and POLY3 workspaces;
                    plot pH-Eh or various property diagrams.

    3 -- Open an existing POLY3 file created by POURBAIX Module
           and make another POURBAIX diagram calculation.
              i.e., open the old GES and POLY3 workspaces;
                    adopt the defined chemical system;
                    modify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.

    4 -- Open an existing POLY3 file created by POURBAIX Module
            (from a previous POURBAIX calculation Option 1 or 3
              or  a previous STEPPING calculation Option 4),
           and make a normal STEPPING calculation.
              i.e., open the old GES and POLY3 workspaces;
                    adopt the defined chemical system;
                    specify one of the T-P-X conditions
                             as the stepping variable;
                    calculate the initial equilibria;
                    perform the stepping calculation;
                    plot various property diagrams.

Select option /1/:
    1 -- Make a completely new POURBAIX diagram calculation
           and automatically plot a pH-Eh diagram.
              i.e., define a new chemical system;
                    specify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.

Consider the GAS phase in calculating a Pourbaix diagram? /Y/:
    You may optionally choose to ignore the GAS mixture phase
    on a calculated/plotted Pourbaix diagram. However, such a
    plot is actually not a complete Pourbaix diagram, due to
    that the thermodynamically-stable phase boundaries between
    the AQUEOUS solution phase and GAS mixture phase will not
    be calculated at all.

    ----------------------------------------------------------
    ** By Y(y), GAS mixture phase shall be always considered;
    ** By N(n), GAS mixture phase will be completely ignored.
    ----------------------------------------------------------

Consider the GAS phase in calculating a Pourbaix diagram? /Y/:
Use single database? /Y/: Combined Database: /PAQ2/:  THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Public Aqueous Soln (SIT) TDB v2
```

```
 H                       O                       ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                DIAMOND_A4              FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                CUB_A13                 CHI_A12
 FE4N                    FECN_CHI  REJECTED
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 PI  REJECTED
 FE3C                    NI3C                    CR3C2
 CR7C3                   CR23C6  REJECTED
 COCO3                   FECO3                   NAHCO3
 NA2CO3                  NA2CO3_S2               NICO3
 CRC6O6  REJECTED
 CO3N                    CRN                     CR2N
 FE2N                    NI3N  REJECTED
 NANO2                   NANO2_S2                NANO3
   REJECTED
 COCL2                   CRCL2                   CRCL3
 FECL2                   FECL3                   NICL2
   REJECTED
 FECLO                   NACLO4                  NACLO4_S2
   REJECTED

 DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION:
 ============================================================
 Normally a POURBAIX diagram and related equilibrium property
 in a heterogeneous interaction system are calculated under a
 certain bulk composition which is usually 1 kg of water with
 defined amounts of dissolving solute substances. The solutes
 may either be completely dissolved into the aqueous solution,
 or be partially dissolved and simultaneously form some solid
 phases.

 CHEMICAL SYSTEM (ELEMENTS):
    Default defined elements  (solvent  H2O):     H  &  O
            and specially assigned ZE(electron) & VA(vacancy).
    Prompt specified elements (solutes  ELEM):
            C   N   S   Cl  Na  Fe  Ni  Co  Cr
 INITIAL BULK COMPOSITION:
    Default defined composition  (solvent):    1.0 kg of H2O
    Prompt specified composition (solutes):    x mole of ELEM
 ------------------------------------------------------------
 Notes: For accepting a default value, just RETURN at prompt;
        For changing to a specific value, enter it at prompt.

 ============================================================
 IMPORTANT NOTE for Entering Solutes in Chemical Formulas:
   First element letter in UPPER case, and second lower case!
     such as  NaCl  CO2  CoCl3  Fe0.93S  NaSO4-1  H2SO4
 ------------------------------------------------------------
   Mass of Water (weight) = 1 kg

   First solute:     Molality of Fe (mole/kg) /.001/:    Second solute:   Next solute:

 ------------------------------------------------------------
 Defined chemical system and initial bulk composition:
    Note: Solutes have been split up into chemical elements
          and their mole numbers. If confirmed, the POURBAIX
          Module will, in further steps, count the initial
          bulk composition in terms of chemical elements.
 ------------------------------------------------------------
         H2O           1.00000000       kg
         ZE           (specially assigned)
          FE          0.1000000000E-02  mole
          CL          0.1000000000E+00  mole
          NA          0.1000000000E+00  mole

Confirm defined system and initial bulk composition? /Y/:

RETRIEVE THERMODYNAMIC DATA FROM THE DATABASE:  PAQ2

 H                       O                       ZE
```

```
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                DIAMOND_A4              FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                CUB_A13                 CHI_A12
 FE4N                    FECN_CHI  REJECTED
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 PI  REJECTED
 FE3C                    NI3C                    CR3C2
 CR7C3                   CR23C6  REJECTED
 COCO3                   FECO3                   NAHCO3
 NA2CO3                  NA2CO3_S2               NICO3
 CRC6O6  REJECTED
 CO3N                    CRN                     CR2N
 FE2N                    NI3N  REJECTED
 NANO2                   NANO2_S2                NANO3
   REJECTED
 COCL2                   CRCL2                   CRCL3
 FECL2                   FECL3                   NICL2
   REJECTED
 FECLO                   NACLO4                  NACLO4_S2
   REJECTED
 REINITIATING GES5 .....
 FE  DEFINED
 CL  DEFINED
 NA  DEFINED
 /-  DEFINED

 This database has following phases for the defined system

 AQUEOUS:A               REF_ELECTRODE           GAS:G
 FCC_A1                  BCC_A2                  HCP_A3
 HALITE                  WUSTITE                 MAGNETITE
 HEMATITE                FE2O3_GAMMA             FEO2H2
 FEO3H3                  FEOOH                   FE2O2O2H2
 NAO2                    NA2O                    NA2O_S2
 NA2O_S3                 NA2O2                   NA2O2_S2
 NAOH                    NAOH_S2                 NA2FEO2

Reject phase(s) /NONE/: Restore phase(s): /NONE/:
 ......................................................

    The following phases are retained in this system:

 AQUEOUS:A               REF_ELECTRODE           GAS:G
 FCC_A1                  BCC_A2                  HCP_A3
 HALITE                  WUSTITE                 MAGNETITE
 HEMATITE                FE2O3_GAMMA             FEO2H2
 FEO3H3                  FEOOH                   FE2O2O2H2
 NAO2                    NA2O                    NA2O_S2
 NA2O_S3                 NA2O2                   NA2O2_S2
 NAOH                    NAOH_S2                 NA2FEO2

 ......................................................

OK? /Y/:  ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
      -Cl system.'
  'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
```

```
      -Cr-Na-Ni-C-H-O-N-S-Cl system.'
  'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
      -Na-Ni-C-H-O-N-S-Cl system.'
  'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
      only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
      from TCAQ2 which covers totally 83 elements and contains many more
      aqueous solution species.'
 -OK-
Should any phase have a miscibility gap check? /N/:
      ...... Reinitializing POLY3 workspaces ......

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, N(CL)=0.1, N(FE)=1E-3,
    N(NA)=0.1
 DEGREES OF FREEDOM 0

Confirm defined conditions? /Y/:
 Calculating start points; please be patient!

 Testing result with global minimization

LIST THE FIRST DEFAULT STARTING EQUILIBRIUM POINT:

 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 T=298.15, P=1E5, B(H2O)=1000, N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.21034, MUR(ZE)=86837
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.57096E+01,  Mass in grams  1.00590E+03
 Total Gibbs energy -1.70696E+07,  Enthalpy -1.59069E+07,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 CL                      1.0000E-01  1.7950E-03 2.2745E-15 -8.3584E+04 SER
 FE                      1.0000E-03  1.7950E-05 1.1996E-62 -3.5345E+05 SER
 H+1                    -2.8715E-03 -5.1544E-05 1.0000E-04 -2.2832E+04 SER
 NA                      1.0000E-01  1.7950E-03 1.0966E-65 -3.7079E+05 SER
 H2O                     5.5508E+01  9.9639E-01 9.9593E-01 -1.0117E+01 AQUEOUS
 ZE                      3.0000E-03  5.3851E-05 1.6334E+15  8.6837E+04 REF_ELEC

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5707E+01, Mass 1.0058E+03, Volume fraction 0.0000E+00  Mole fractions:
 H2O  9.96407E-01  NA   1.79510E-03  FE   8.00000E-12
 CL   1.79510E-03  H+1  2.30784E-06  ZE  -1.85327E-10
 Constitution:           SiteFraction    Molality      Activity      log10Act
 H2O                     9.96407E-01   5.55084E+01   9.96010E-01    -0.0017
 CL-1                    1.79510E-03   1.00003E-01   7.76714E-02    -1.1097
 NA+1                    1.79510E-03   1.00003E-01   7.76714E-02    -1.1097
 H+1                     2.30800E-06   1.28575E-04   1.00000E-04    -4.0000
 O2                      2.77253E-11   1.54453E-09   1.54441E-09    -8.8112
 OH-1                    2.31700E-12   1.29077E-10   1.00217E-10    -9.9991
 O3                      1.00000E-12   0.00000E+00   3.88137E-40   -39.4110
 HCLO                    1.00000E-12   0.00000E+00   8.75924E-18   -17.0575
 H2O2                    1.00000E-12   0.00000E+00   8.94229E-22   -21.0486
 HCLO2                   1.00000E-12   0.00000E+00   8.41611E-36   -35.0749
 H2                      1.00000E-12   0.00000E+00   2.21838E-42   -41.6540
 HO2-1                   1.00000E-12   0.00000E+00   1.89240E-29   -28.7230
 FEOH+2                  1.00000E-12   0.00000E+00   9.27037E-13   -12.0329
 FEOH+1                  1.00000E-12   0.00000E+00   1.26848E-19   -18.8967
 FEO3H3-1                1.00000E-12   0.00000E+00   1.08151E-66   -65.9660
 FECL+2                  1.00000E-12   0.00000E+00   3.39784E-14   -13.4688
 FE2O2H2+4               1.00000E-12   0.00000E+00   3.71406E-23   -22.4302
 FE+3                    1.00000E-12   0.00000E+00   1.53892E-14   -13.8128
```

```
 FE+2                    1.00000E-12   0.00000E+00   8.04440E-17   -16.0945
 CLO4-1                  1.00000E-12   0.00000E+00   3.24705E-35   -34.4885
 CLO3-1                  1.00000E-12   0.00000E+00   2.33976E-32   -31.6308
 CLO2-1                  1.00000E-12   0.00000E+00   8.80835E-34   -33.0551
 CLO2                    1.00000E-12   0.00000E+00   1.56010E-36   -35.8068
 CLO-1                   1.00000E-12   0.00000E+00   1.89890E-21   -20.7215
 CL2                     1.00000E-12   0.00000E+00   1.43332E-19   -18.8437
 Solution Properties:   pH =   4.0000    Eh =    0.9000 V     I =   0.1001
                        pe =  15.2131    Ah =   86.8370 kJ   m* =   0.2001
                        Aw =   0.9960    Os =    1.1089
                        At1= 1.0000E-12  At2= 1.3008E-10 (equiv_mol/kg_H2O)

 HEMATITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 2.5000E-03, Mass 7.9847E-02, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.20000E+00  FE   4.00000E-01  NA   0.00000E+00
 H2O  6.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00
 Constitution:
 FE2O3  1.00000E+00

LIST THE DEFINED SYMBOLS:
 DEFINED CONSTANTS
    TSLIMIT0=99, AH2O=55.508435, WH2O=1.80152E-2, RNL=2.3025851, R=8.31451,
       RNF=96485.309
 DEFINED FUNCTIONS AND VARIABLES%
    TC%=T-273.15
    PBAR%=P*1E-05
    PKB%=P*1E-08
    RT%=R*T
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1) )
    YH2O=Y(AQUEOUS,H2O)
    ACRH2O=ACR(H2O,AQUEOUS)
    RCH2O=ACR(H2O,AQUEOUS)
    MLH2O=AH2O
    ACTW=ACRH2O
    OSMC=-YH2O/ (1-YH2O )* LOG(ACRH2O )
    TMI= (1-YH2O )*AH2O/YH2O
    AHZE=MUR(ZE)/1000
    PEZE=MUR(ZE)/ (RNL*RT )
    AI1=ACR(CL-1,AQUEOUS)*AH2O
    RC1=ACR(CL-1,AQUEOUS)*YH2O/Y(AQUEOUS,CL-1)
    ML1=Y(AQUEOUS,CL-1)*AH2O/YH2O
    AI2=ACR(CL2,AQUEOUS)*AH2O
    RC2=ACR(CL2,AQUEOUS)*YH2O/Y(AQUEOUS,CL2)
    ML2=Y(AQUEOUS,CL2)*AH2O/YH2O
    AI3=ACR(CLO-1,AQUEOUS)*AH2O
    RC3=ACR(CLO-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO-1)
    ML3=Y(AQUEOUS,CLO-1)*AH2O/YH2O
    AI4=ACR(CLO2,AQUEOUS)*AH2O
    RC4=ACR(CLO2,AQUEOUS)*YH2O/Y(AQUEOUS,CLO2)
    ML4=Y(AQUEOUS,CLO2)*AH2O/YH2O
    AI5=ACR(CLO2-1,AQUEOUS)*AH2O
    RC5=ACR(CLO2-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO2-1)
    ML5=Y(AQUEOUS,CLO2-1)*AH2O/YH2O
    AI6=ACR(CLO3-1,AQUEOUS)*AH2O
    RC6=ACR(CLO3-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO3-1)
    ML6=Y(AQUEOUS,CLO3-1)*AH2O/YH2O
    AI7=ACR(CLO4-1,AQUEOUS)*AH2O
    RC7=ACR(CLO4-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO4-1)
    ML7=Y(AQUEOUS,CLO4-1)*AH2O/YH2O
    AI8=ACR(FE+2,AQUEOUS)*AH2O
    RC8=ACR(FE+2,AQUEOUS)*YH2O/Y(AQUEOUS,FE+2)
    ML8=Y(AQUEOUS,FE+2)*AH2O/YH2O
    AI9=ACR(FE+3,AQUEOUS)*AH2O
    RC9=ACR(FE+3,AQUEOUS)*YH2O/Y(AQUEOUS,FE+3)
    ML9=Y(AQUEOUS,FE+3)*AH2O/YH2O
    AI10=ACR(FE2O2H2+4,AQUEOUS)*AH2O
    RC10=ACR(FE2O2H2+4,AQUEOUS)*YH2O/Y(AQUEOUS,FE2O2H2+4)
    ML10=Y(AQUEOUS,FE2O2H2+4)*AH2O/YH2O
    AI11=ACR(FECL+2,AQUEOUS)*AH2O
    RC11=ACR(FECL+2,AQUEOUS)*YH2O/Y(AQUEOUS,FECL+2)
    ML11=Y(AQUEOUS,FECL+2)*AH2O/YH2O
    AI12=ACR(FEO3H3-1,AQUEOUS)*AH2O
    RC12=ACR(FEO3H3-1,AQUEOUS)*YH2O/Y(AQUEOUS,FEO3H3-1)
```

```
   ML12=Y(AQUEOUS,FEO3H3-1)*AH2O/YH2O
   AI13=ACR(FEOH+1,AQUEOUS)*AH2O
   RC13=ACR(FEOH+1,AQUEOUS)*YH2O/Y(AQUEOUS,FEOH+1)
   ML13=Y(AQUEOUS,FEOH+1)*AH2O/YH2O
   AI14=ACR(FEOH+2,AQUEOUS)*AH2O
   RC14=ACR(FEOH+2,AQUEOUS)*YH2O/Y(AQUEOUS,FEOH+2)
   ML14=Y(AQUEOUS,FEOH+2)*AH2O/YH2O
   AI15=ACR(H+1,AQUEOUS)*AH2O
   RC15=ACR(H+1,AQUEOUS)*YH2O/Y(AQUEOUS,H+1)
   ML15=Y(AQUEOUS,H+1)*AH2O/YH2O
   AI16=ACR(H2,AQUEOUS)*AH2O
   RC16=ACR(H2,AQUEOUS)*YH2O/Y(AQUEOUS,H2)
   ML16=Y(AQUEOUS,H2)*AH2O/YH2O
   AI17=ACR(H2O,AQUEOUS)
   RC17=ACR(H2O,AQUEOUS)/Y(AQUEOUS,H2O)
   ML17=Y(AQUEOUS,H2O)*AH2O/YH2O
   AI18=ACR(H2O2,AQUEOUS)*AH2O
   RC18=ACR(H2O2,AQUEOUS)*YH2O/Y(AQUEOUS,H2O2)
   ML18=Y(AQUEOUS,H2O2)*AH2O/YH2O
   AI19=ACR(HCLO,AQUEOUS)*AH2O
   RC19=ACR(HCLO,AQUEOUS)*YH2O/Y(AQUEOUS,HCLO)
   ML19=Y(AQUEOUS,HCLO)*AH2O/YH2O
   AI20=ACR(HCLO2,AQUEOUS)*AH2O
   RC20=ACR(HCLO2,AQUEOUS)*YH2O/Y(AQUEOUS,HCLO2)
   ML20=Y(AQUEOUS,HCLO2)*AH2O/YH2O
   AI21=ACR(HO2-1,AQUEOUS)*AH2O
   RC21=ACR(HO2-1,AQUEOUS)*YH2O/Y(AQUEOUS,HO2-1)
   ML21=Y(AQUEOUS,HO2-1)*AH2O/YH2O
   AI22=ACR(NA+1,AQUEOUS)*AH2O
   RC22=ACR(NA+1,AQUEOUS)*YH2O/Y(AQUEOUS,NA+1)
   ML22=Y(AQUEOUS,NA+1)*AH2O/YH2O
   AI23=ACR(O2,AQUEOUS)*AH2O
   RC23=ACR(O2,AQUEOUS)*YH2O/Y(AQUEOUS,O2)
   ML23=Y(AQUEOUS,O2)*AH2O/YH2O
   AI24=ACR(O3,AQUEOUS)*AH2O
   RC24=ACR(O3,AQUEOUS)*YH2O/Y(AQUEOUS,O3)
   ML24=Y(AQUEOUS,O3)*AH2O/YH2O
   AI25=ACR(OH-1,AQUEOUS)*AH2O
   RC25=ACR(OH-1,AQUEOUS)*YH2O/Y(AQUEOUS,OH-1)
   ML25=Y(AQUEOUS,OH-1)*AH2O/YH2O
   IS1=.5*ML1+.5*ML3+.5*ML5
   IS2=.5*ML6+.5*ML7+.5*ML8*2**2
   IS3=.5*ML9*3**2+.5*ML10*4**2+.5*ML11*2**2
   IS4=.5*ML12+.5*ML13+.5*ML14*2**2
   IS5=.5*ML15+.5*ML21+.5*ML22
   ISTR=1*IS1+1*IS2+1*IS3+1*IS4+1*IS5
   RLOGH= LOG10(ACR(H+1,AQUEOUS)*AH2O )
   RLOGOH= LOG10(ACR(OH-1,AQUEOUS)*AH2O )
   RLOGH2O= LOG10(ACR(H2O,AQUEOUS) )
DEFINED TABLES
   GPT=T, P, PH, EH, ISTR
   SFT=Y(AQUEOUS,CL-1), Y(AQUEOUS,CL2), Y(AQUEOUS,CLO-1), Y(AQUEOUS,CLO2),
      Y(AQUEOUS,CLO2-1), Y(AQUEOUS,CLO3-1), Y(AQUEOUS,CLO4-1),
      Y(AQUEOUS,FE+2), Y(AQUEOUS,FE+3), Y(AQUEOUS,FE2O2H2+4),
      Y(AQUEOUS,FECL+2), Y(AQUEOUS,FEO3H3-1), Y(AQUEOUS,FEOH+1),
      Y(AQUEOUS,FEOH+2), Y(AQUEOUS,H+1), Y(AQUEOUS,H2), Y(AQUEOUS,H2O),
      Y(AQUEOUS,H2O2), Y(AQUEOUS,HCLO), Y(AQUEOUS,HCLO2), Y(AQUEOUS,HO2-1),
      Y(AQUEOUS,NA+1), Y(AQUEOUS,O2), Y(AQUEOUS,O3), Y(AQUEOUS,OH-1), PH, EH
   AYT=AC(CL-1,AQUEOUS), AC(CL2,AQUEOUS), AC(CLO-1,AQUEOUS),
      AC(CLO2,AQUEOUS), AC(CLO2-1,AQUEOUS), AC(CLO3-1,AQUEOUS),
      AC(CLO4-1,AQUEOUS), AC(FE+2,AQUEOUS), AC(FE+3,AQUEOUS),
      AC(FE2O2H2+4,AQUEOUS), AC(FECL+2,AQUEOUS), AC(FEO3H3-1,AQUEOUS),
      AC(FEOH+1,AQUEOUS), AC(FEOH+2,AQUEOUS), AC(H+1,AQUEOUS),
      AC(H2,AQUEOUS), AC(H2O,AQUEOUS), AC(H2O2,AQUEOUS), AC(HCLO,AQUEOUS),
      AC(HCLO2,AQUEOUS), AC(HO2-1,AQUEOUS), AC(NA+1,AQUEOUS), AC(O2,AQUEOUS),
      AC(O3,AQUEOUS), AC(OH-1,AQUEOUS), PH, EH
   ART=ACR(CL-1,AQUEOUS), ACR(CL2,AQUEOUS), ACR(CLO-1,AQUEOUS),
      ACR(CLO2,AQUEOUS), ACR(CLO2-1,AQUEOUS), ACR(CLO3-1,AQUEOUS),
      ACR(CLO4-1,AQUEOUS), ACR(FE+2,AQUEOUS), ACR(FE+3,AQUEOUS),
      ACR(FE2O2H2+4,AQUEOUS), ACR(FECL+2,AQUEOUS), ACR(FEO3H3-1,AQUEOUS),
      ACR(FEOH+1,AQUEOUS), ACR(FEOH+2,AQUEOUS), ACR(H+1,AQUEOUS),
      ACR(H2,AQUEOUS), ACR(H2O,AQUEOUS), ACR(H2O2,AQUEOUS),
      ACR(HCLO,AQUEOUS), ACR(HCLO2,AQUEOUS), ACR(HO2-1,AQUEOUS),
      ACR(NA+1,AQUEOUS), ACR(O2,AQUEOUS), ACR(O3,AQUEOUS), ACR(OH-1,AQUEOUS),
```

```
       PH, EH
    AIT=AI1, AI2, AI3, AI4, AI5, AI6, AI7, AI8, AI9, AI10, AI11, AI12, AI13,
       AI14, AI15, AI16, AI17, AI18, AI19, AI20, AI21, AI22, AI23, AI24, AI25,
       PH, EH
    RCT=RC1, RC2, RC3, RC4, RC5, RC6, RC7, RC8, RC9, RC10, RC11, RC12, RC13,
       RC14, RC15, RC16, RC17, RC18, RC19, RC20, RC21, RC22, RC23, RC24, RC25,
       PH, EH
    MLT=ML1, ML2, ML3, ML4, ML5, ML6, ML7, ML8, ML9, ML10, ML11, ML12, ML13,
       ML14, ML15, ML16, ML18, ML19, ML20, ML21, ML22, ML23, ML24, ML25, ISTR,
       PH, EH

LIST THE DEFINED AXIS-VARIABLES:

  Axis No 1: LNACR(H+1)            Min: -32.22994 Max: 0         Inc: 0.8
  Axis No 2: MUR(ZE)               Min: -150000   Max: 200000    Inc: 8600

     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 equivalent to 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 0.09 (V)

           The maximum pH limit has actually been calculated
           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.

     IMPORTANT FACTS: The default definitions of the pH and Eh
         quantities in the POURBAIX-Module are always as below:
           pH = -log10ACR(H+1)
           Eh = MUR(ZE)/RNF
         where RNF is the Faraday constant (96485.309 C/mol),
         MUR(ZE) is the chemical potential of electron (w.r.t.
         the standard hydrogen electrode, and ACR(H+1) is the
         activity of H+1 system-component (under the reference
         state of SER that is always the default settings in the
         POURBAIX-Module calculations).

     Please also notice that: the default pH definition shown
         above is absolutely equivalent to the conventional
         definition of acidity:
           pH = -log10ACR(H+1,AQUEOUS)
         which shall be valid and applied ONLY if there has been
         a simultaneous definition of the reference state for the
         H+1 system-component as the H+1 cation species in the
         AQUEOUS solution phase under current temperature (*)
         and 100000 Pascal (i.e., 1 bar).

Accept the default settings for two mapping variables? /Y/:
 Testing result with global minimization

LIST ALL THE INITIAL EQUILIBRIA FOR MAPPING:

 No 1  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.10000002,
    N(FE)=1.0000125E-3, N(NA)=0.1, LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 2  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.10000002,
    N(FE)=1.0000125E-3, N(NA)=0.1, LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 3  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.10000002,
    N(FE)=1.0000125E-3, N(NA)=0.1, LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 4  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.10000002,
    N(FE)=1.0000125E-3, N(NA)=0.1, LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 5  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.10000008,
    N(FE)=1.0000149E-3, N(NA)=0.1, LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 6  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.10000008,
    N(FE)=1.0000149E-3, N(NA)=0.1, LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 7  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.10000008,
    N(FE)=1.0000149E-3, N(NA)=0.1, LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 8  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.10000008,
    N(FE)=1.0000149E-3, N(NA)=0.1, LNACR(H+1)=-16.118096, MUR(ZE)=100.

 MAP THE POURBAIX DIAGRAM:
 Version S mapping is selected
```

```
 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Working hard
 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16

 Phase region boundary   1 at:  -9.210E+00  9.529E+04
  ** GAS
     AQUEOUS
     HEMATITE
 *** Buffer saved on file: POURBAIX.POLY3
 Calculated..           30  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:  -3.223E+01  3.827E+04
  ** GAS
     AQUEOUS
     HEMATITE
 Calculated.           39  equilibria

 Phase region boundary   3 at:  -1.975E+00  1.132E+05
  ** GAS
     AQUEOUS
  ** HEMATITE

 Phase region boundary   4 at:  -1.975E+00  1.132E+05
  ** GAS
     AQUEOUS
 Calculated..            4  equilibria
 Terminating at axis limit.

       :
       :
       :

 Phase region boundary  26 at:  -1.612E+01 -2.701E+04
     AQUEOUS
     HEMATITE
  ** MAGNETITE
 Calculated..           22  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  27 at:  -1.612E+01 -2.701E+04
     AQUEOUS
     HEMATITE
  ** MAGNETITE
 Calculated.            4  equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:  -1.116E+01  1.000E+02
     AQUEOUS
  ** HEMATITE
 Calculated.            6  equilibria
```

```
Terminating at known equilibrium

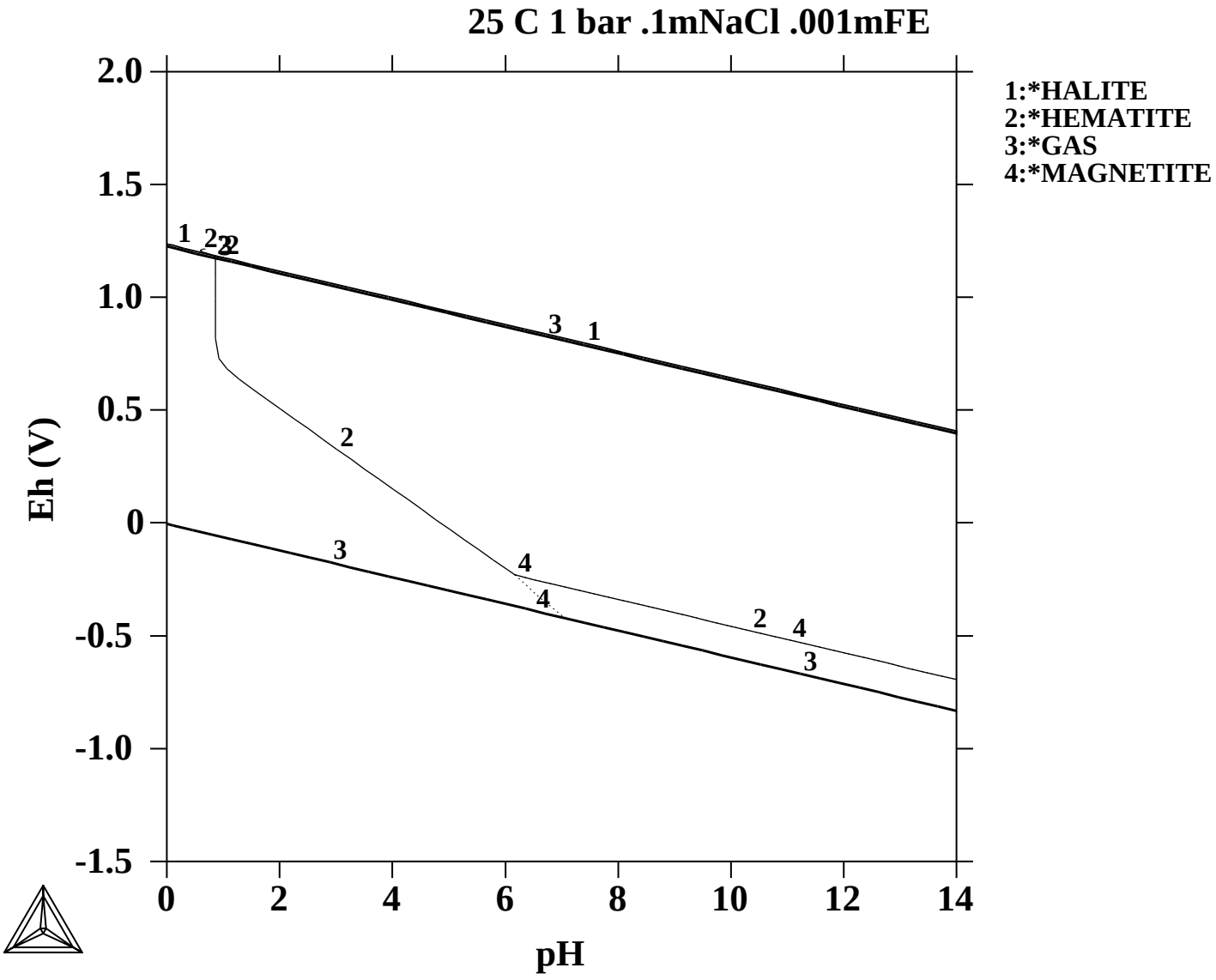
Phase region boundary  29 at:  -1.116E+01  1.000E+02
    AQUEOUS
 ** HEMATITE
Calculated.           22  equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: POURBAIX.POLY3
CPU time for mapping        2965  seconds

 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

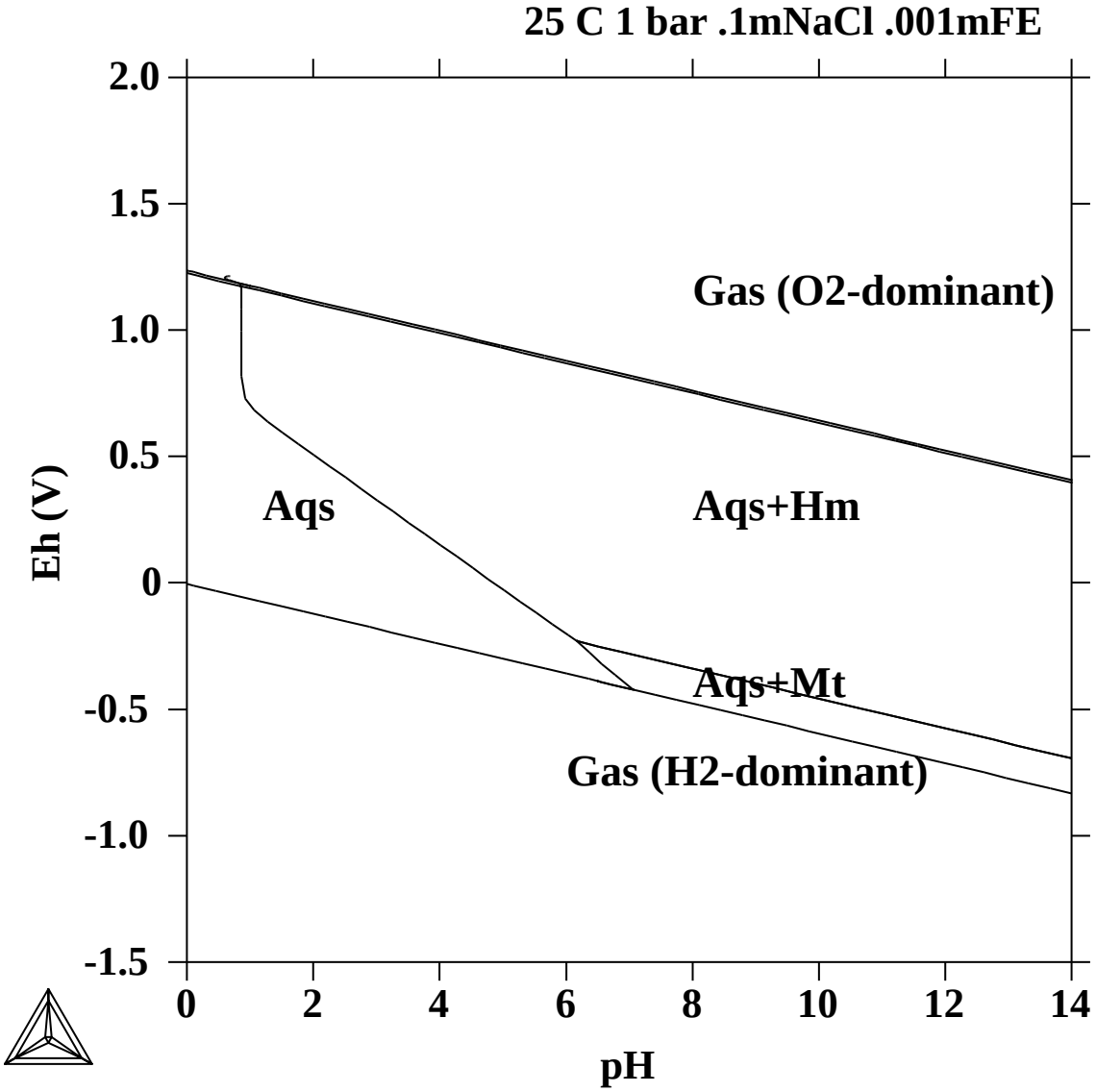
Setting automatic diagram axis

Plotting the diagram; please be patient!
```

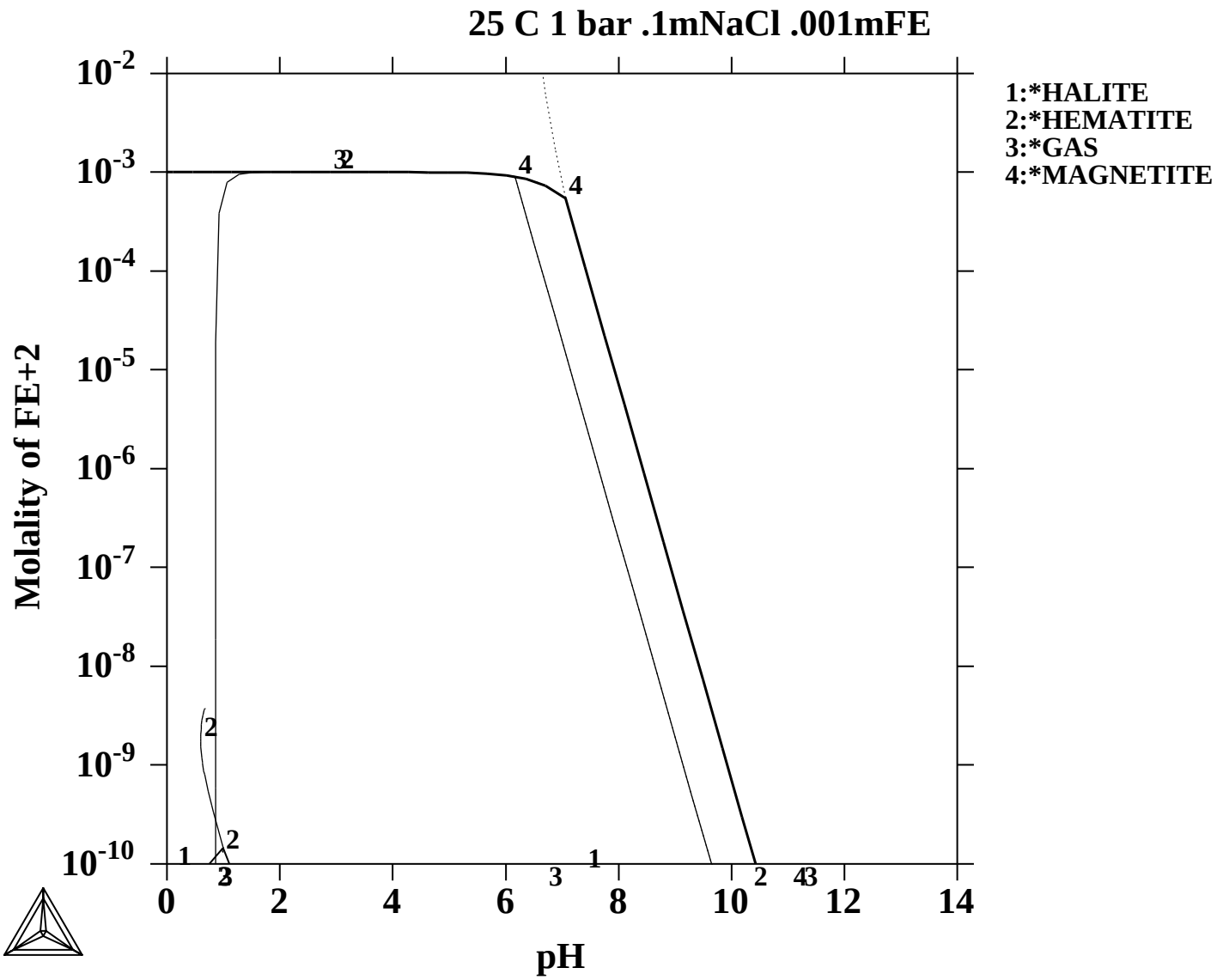
THERMO-CALC (2009.04.29:16.21) :Pourbaix Diagram



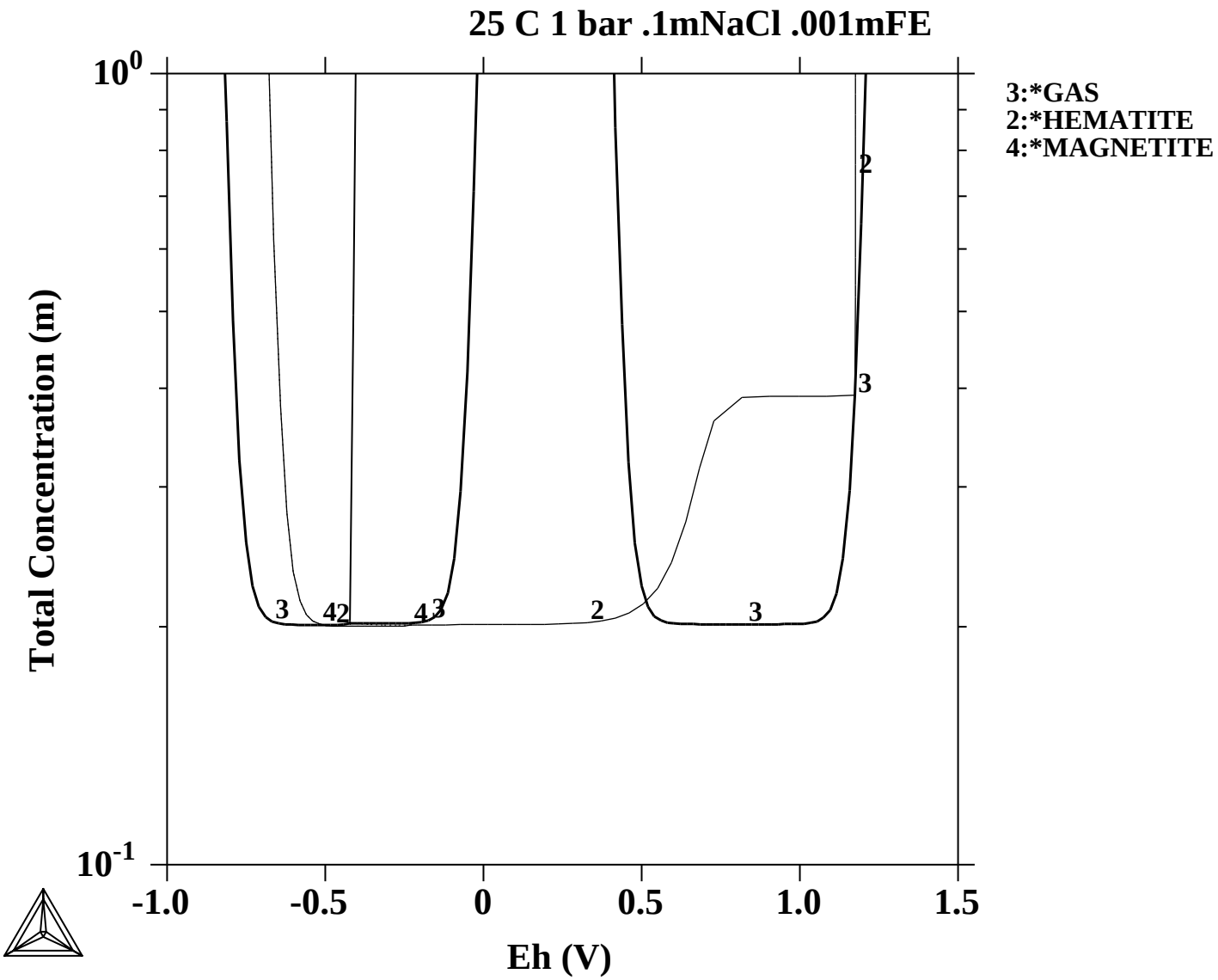
THERMO-CALC (2009.04.29:16.21) :Pourbaix Diagram



THERMO-CALC (2009.04.29:16.21) :Property Diagram



THERMO-CALC (2009.04.29:16.23) :Property Diagram



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Calculation
of a solubility product

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of a solubility product
SYS: @@
SYS: set-log ex41,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/:  tcfe6
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .19
2nd alloying element: mn 1.16
Next alloying element: si .2
Next alloying element: cr .72
Next alloying element: ni .2
Next alloying element: mo .08
Next alloying element: cu .26
Next alloying element: al .027
Next alloying element: n .0089
Next alloying element:
Temperature (C) /1000/:  1056
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MO  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CU  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 AL  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 N  DEFINED

 This database has following phases for the defined system

 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M6C                     M5C2
 M3C2                    MC_ETA                  MC_SHP
 KSI_CARBIDE             A1_KAPPA                KAPPA
 Z_PHASE                 FE4N_LP1                FECN_CHI
```

```
 PI                      SIGMA                   MU_PHASE
 P_PHASE                 R_PHASE                 CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   NI3TI                   AL4C3
 FE8SI2C                 SIC                     ALN

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE
 ..................................................

    The following phases are retained in this system:

 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  DIAMOND_FCC_A4
 GRAPHITE                CEMENTITE               M23C6
 M7C3                    M6C                     M5C2
 M3C2                    MC_ETA                  MC_SHP
 KSI_CARBIDE             A1_KAPPA                KAPPA
 Z_PHASE                 FE4N_LP1                FECN_CHI
 PI                      SIGMA                   MU_PHASE
 P_PHASE                 R_PHASE                 CHI_A12
 LAVES_PHASE_C14         M3SI                    CR3SI
 FE2SI                   MSI                     M5SI3
 NBNI3                   NI3TI                   AL4C3
 FE8SI2C                 SIC                     ALN

 ..................................................

OK? /Y/: Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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  'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
  'I. Ansara, unpublished work (1991); Cr-Si'
  'A. Bolcavage and U.R. Kattner, J. Phase Equil., 2, (1996); Nb-Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Halite'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
 Calculated        29482  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3:
POLY_3: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6
```

```
 Conditions:
 T=1329.15, W(C)=1.9E-3, W(MN)=1.16E-2, W(SI)=2E-3, W(CR)=7.2E-3, W(NI)=2E-3,
    W(MO)=8E-4, W(CU)=2.6E-3, W(AL)=2.7E-4, W(N)=8.9E-5, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1329.15 K (  1056.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53245E+01
 Total Gibbs energy -6.89274E+04,  Enthalpy  3.91105E+04,  Volume  7.33489E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      5.5361E-04  2.7000E-04 1.1877E-09 -2.2712E+05 SER
 C                       8.7517E-03  1.9000E-03 8.6212E-03 -5.2532E+04 SER
 CR                      7.6609E-03  7.2000E-03 7.6344E-05 -1.0477E+05 SER
 CU                      2.2636E-03  2.6000E-03 9.9901E-05 -1.0180E+05 SER
 FE                      9.6245E-01  9.7154E-01 2.2984E-03 -6.7142E+04 SER
 MN                      1.1682E-02  1.1600E-02 1.1088E-05 -1.2609E+05 SER
 MO                      4.6133E-04  8.0000E-04 9.9163E-06 -1.2732E+05 SER
 N                       3.5153E-04  8.9000E-05 2.4129E-07 -1.6839E+05 SER
 NI                      1.8853E-03  2.0000E-03 2.7231E-06 -1.4161E+05 SER
 SI                      3.9396E-03  2.0000E-03 5.2424E-09 -2.1071E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.9950E-01, Mass 5.5314E+01, Volume fraction 9.9957E-01  Mass fractions:
 FE  9.71720E-01  CU  2.60048E-03  C   1.90035E-03  N   2.61245E-05
 MN  1.16021E-02  SI  2.00037E-03  MO  8.00147E-04
 CR  7.20133E-03  NI  2.00037E-03  AL  1.48900E-04

 ALN                         Status ENTERED     Driving force  0.0000E+00
 Moles 4.9673E-04, Mass 1.0180E-02, Volume fraction 4.3238E-04  Mass fractions:
 AL  6.58274E-01  NI  0.00000E+00  FE  0.00000E+00  C   0.00000E+00
 N   3.41726E-01  MO  0.00000E+00  CU  0.00000E+00
 SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: def-dia
   ... the command in full is DEFINE_DIAGRAM
Same elements as before? /Y/:  Y
 For binary or ternary diagrams you may prefer the special modules

 You must specify a value for all compositions and the temperature even
 if you want to use it as axis.
Mass (weight) percent of AL /.027/:  .027
Mass (weight) percent of C /.19/:  .19
Mass (weight) percent of CR /.72/:  .72
Mass (weight) percent of CU /.26/:  .26
Mass (weight) percent of MN /1.16/:  1.16
Mass (weight) percent of MO /.08/:  .08
Mass (weight) percent of N /.0089/:  .0089
Mass (weight) percent of NI /.2/:  .2
Mass (weight) percent of SI /.2/:  .2
Temperature (C) /1056/:  1056
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
 You must now set an independent axis for your diagram
 as one of the following conditions:
 Condition  1 is temperature (Celsius)
 Condition  2 is mass percent of C
 Condition  3 is mass percent of MN
 Condition  4 is mass percent of SI
 Condition  5 is mass percent of CR
 Condition  6 is mass percent of NI
 Condition  7 is mass percent of MO
 Condition  8 is mass percent of CU
 Condition  9 is mass percent of AL
 Condition 10 is mass percent of N
Give the number of the condition to vary /1/:  1
Minimum value (C) /800/:  650
Maximum value (C) /1800/:  1200
 The second axis can be another of the conditions above and you will then
 calculate a phase diagram.
 Or you may want to plot how some other quantities depend on the selected
 condition and you will then calculate a  "property" diagram.
```

```
 In addition to the conditions above you may use these selected
 dependent quantities on the vertical axis:
 Dependent 11 is mass fraction of all phases
 Dependent 12 is composition of a phase
 Dependent 13 is the fraction of a component in all phases
 (In the post processor you may select many other quantities)
Give the number of the quantity on second axis /11/:  11
Save file: /RESULT.POLY3/:  tcex41
 No initial equilibrium, using default
 Step will start from axis value    1329.15
 Global calculation of initial equilibrium ....OK

 Phase Region from    1329.15     for:
     ALN
     FCC_A1#1
 Global test at  1.40915E+03 .... OK
 Global check of removing phase at  1.46358E+03
 Calculated    16 equilibria

 Phase Region from    1463.58     for:
     FCC_A1#1
 Terminating at    1473.15
 Calculated     4 equilibria

 Phase Region from    1329.15     for:
     ALN
     FCC_A1#1
 Global test at  1.24915E+03 .... OK
 Global test at  1.14915E+03 .... OK
 Global check of adding phase at  1.07226E+03
 Calculated    28 equilibria

 Phase Region from    1072.26     for:
     ALN
     BCC_A2
     FCC_A1#1
 Global test at  9.99150E+02 .... OK
 Global check of adding phase at  9.98515E+02
 Calculated    11 equilibria

       :
       :
       :

 Phase Region from    996.947     for:
     ALN
     BCC_A2
     CEMENTITE
     FCC_A1#1
     M7C3
 Global check of removing phase at  9.95947E+02
 Calculated     3 equilibria

 Phase Region from    995.947     for:
     ALN
     BCC_A2
     CEMENTITE
     FCC_A1#1
 Global check of removing phase at  9.68328E+02
 Calculated     6 equilibria

 Phase Region from    968.328     for:
     ALN
     BCC_A2
     CEMENTITE
 Global check of adding phase at  9.45779E+02
 Calculated     5 equilibria

 Phase Region from    945.779     for:
     ALN
     BCC_A2
     CEMENTITE
     M7C3
```

```
 Terminating at    923.150
 Calculated     6 equilibria
 *** Buffer saved on file: tcex41.POLY3

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is REINITIATE_PLOT_SETTINGS

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

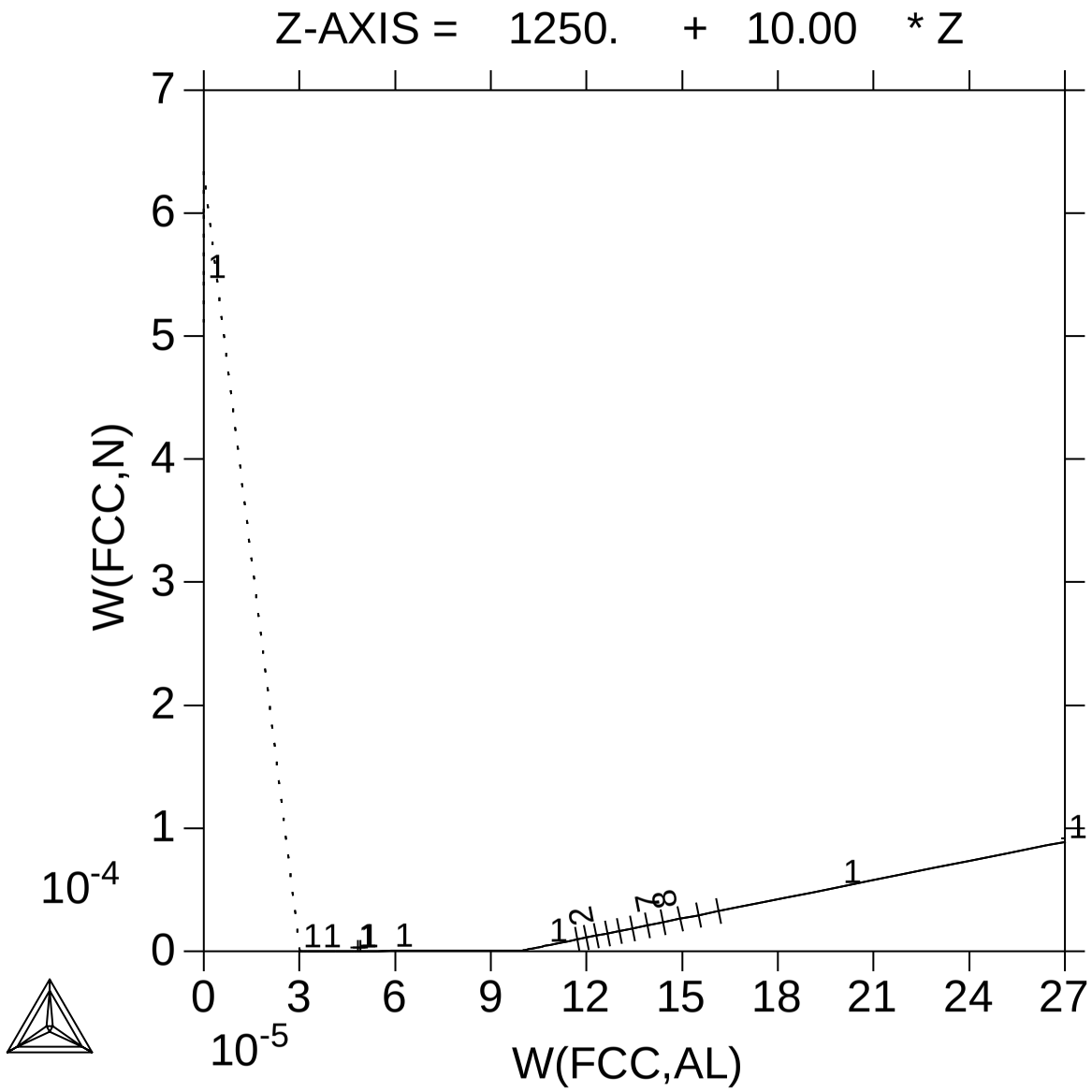
 Setting automatic diagram axis

   ... the command in full is SET_AUTOMATIC_DIAGRAM_A

 Setting automatic diagram axis

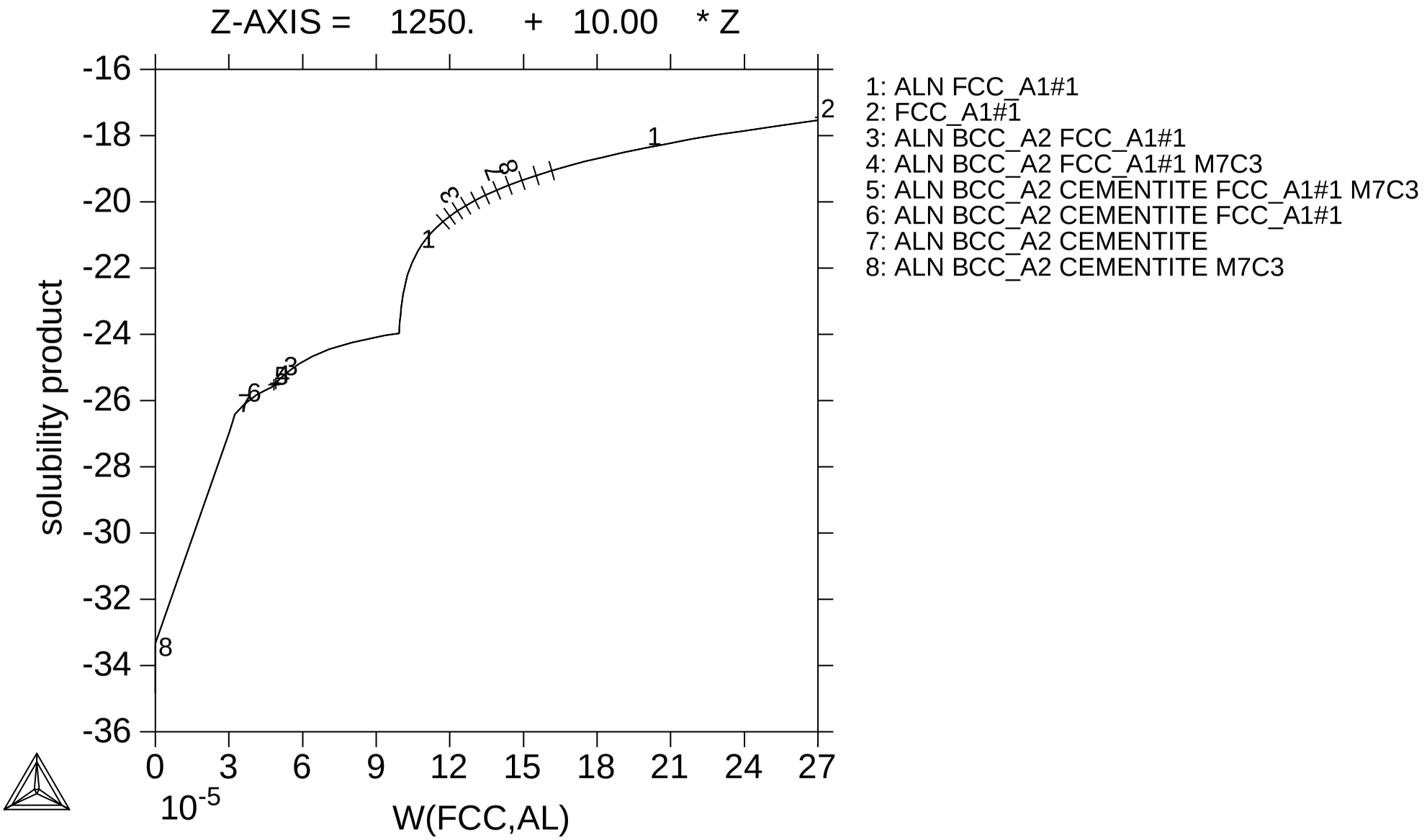
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,,
POST:
POST: s-d-a x w(fcc,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(fcc,n)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-d-a z t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 1250 1350
   ... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 41a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Now let's go back to POLY3 and enter a function
POST: @@ corresponding to the solubillity product
POST: back
POLY_3: enter fun
   ... the command in full is ENTER_SYMBOL
Name: sp
Function: log(w(fcc,al)*w(fcc,n));
POLY_3:
POLY_3: @@ Finally, let's go back to POST and plot the entered function
POLY_3: post
POST:
POST: s-d-a y sp
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-t-s y n solubility product
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: set-title example 41b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
 CPU time          24  seconds
```

THERMO-CALC (2009.04.27:14.36) :example 41a
DATABASE:TCFE6



1:W(FCC_A1#1,AL),W(FCC_A1#1,N)

THERMO-CALC (2009.04.27:14.36) :example 41b
DATABASE:TCFE6



42

Formation of Para-pearlite (Isopleth Calculation)

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Paraequilibrium calculation - Formation of Para-pearlite - Isopleth
SYS: @@
SYS: @@  Fe-Mn-C system at 2.5%Mn Mass u-fraction
SYS: @@
SYS: set-log ex42,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw tcfe6
   ... the command in full is SWITCH_DATABASE
TDB_TCFE6: d-sys fe c mn
   ... the command in full is DEFINE_SYSTEM
 FE                      C                       MN
   DEFINED
TDB_TCFE6: rej ph gra m5c2
   ... the command in full is REJECT
 GRAPHITE                M5C2  REJECTED
TDB_TCFE6: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'P. Franke, estimated parameter within SGTE, 2008; Fe-Mn-C'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
                    :
                    :
                    :
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C-FE-MO'
  'D. Connetable, J. Lacaze, P. Maugis and B. Sundman; Accepted in CALPHAD,
      2008; Al-C-Fe'
  'Thermo-Calc Software (2008): Volume data updated for TCFE6 database (TCFE
      v6, April, 2008).'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'Estimated parameter for solubility of C in Fe4N, 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
 -OK-
TDB_TCFE6: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
```

```
POLY_3: @@
POLY_3: @@ To work with u-fractions, simply set the status of component C to SPECIAL
POLY_3: @@
POLY_3: c-s com c
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: special
POLY_3: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       SPECIAL   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 M7C3                    ENTERED    0.00000000E+00  0.00000000E+00
 M23C6                   ENTERED    0.00000000E+00  0.00000000E+00
 LAVES_PHASE_C14         ENTERED    0.00000000E+00  0.00000000E+00
 KSI_CARBIDE             ENTERED    0.00000000E+00  0.00000000E+00
 KAPPA                   ENTERED    0.00000000E+00  0.00000000E+00
 HCP_A3                  ENTERED    0.00000000E+00  0.00000000E+00
 FECN_CHI                ENTERED    0.00000000E+00  0.00000000E+00
 FE4N_LP1                ENTERED    0.00000000E+00  0.00000000E+00
 FCC_A1                  ENTERED    0.00000000E+00  0.00000000E+00
 DIAMOND_FCC_A4          ENTERED    0.00000000E+00  0.00000000E+00
 CEMENTITE               ENTERED    0.00000000E+00  0.00000000E+00
 BCC_A2                  ENTERED    0.00000000E+00  0.00000000E+00
 LIQUID                  ENTERED    0.00000000E+00  0.00000000E+00
 *** STATUS FOR ALL SPECIES
 C  ENTERED    FE ENTERED    MN ENTERED    VA ENTERED
POLY_3:
POLY_3:@?
POLY_3: s-c t=900 p=1e5 n=1 w(c)=0.002 w(mn)=0.025
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        11623  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=900, P=1E5, N=1, W(C)=2E-3, W(MN)=2.5E-2
 DEGREES OF FREEDOM 0

 Temperature    900.00 K (   626.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.54204E+01
 Total Gibbs energy -3.64282E+04,  Enthalpy  2.02873E+04,  Volume  7.24808E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2099E-03  2.0000E-03 1.8066E-01 -1.2805E+04 SER
 FE                      9.6562E-01  9.7500E-01 8.1690E-03 -3.5974E+04 SER
 MN                      2.5169E-02  2.5000E-02 2.3600E-04 -6.2496E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.6371E-01, Mass 5.3798E+01, Volume fraction 9.6995E-01  Mass fractions:
 FE  9.81636E-01  MN  1.83337E-02  C   3.07634E-05

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 3.6288E-02, Mass 1.6223E+00, Volume fraction 3.0048E-02  Mass fractions:
 FE  6.88481E-01  MN  2.44355E-01  C   6.71647E-02
POLY_3: s-a-v 1 w(c) 0 0.02
   ... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/: 2.5E-04
POLY_3: s-a-v 2 t 800 1200 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex42a y
```

```
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   2.500E-04  8.868E+02
     BCC_A2
     CEMENTITE
  ** FCC_A1
 *** Buffer saved on file: tcex42a.POLY3
 Calculated.            5  equilibria

 Phase region boundary   2 at:   1.756E-05  8.799E+02
     BCC_A2
  ** CEMENTITE
  ** FCC_A1

 Phase region boundary   3 at:   1.756E-05  8.799E+02
     BCC_A2
  ** FCC_A1
 Calculated           18  equilibria

 Phase region boundary   4 at:   1.756E-05  8.799E+02
     BCC_A2
  ** CEMENTITE
 Calculated..          10  equilibria
 Terminating at axis limit.
```

```
      :
      :
      :

 Phase region boundary  34 at:   1.283E-02  1.190E+03
  ** CEMENTITE
     FCC_A1
 Calculated.           34  equilibria
 Terminating at known equilibrium

 Phase region boundary  35 at:   1.283E-02  1.190E+03
  ** CEMENTITE
     FCC_A1
 Calculated..           4  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  36 at:   1.975E-02  9.830E+02
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated.           53  equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   1.975E-02  9.830E+02
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated..           3  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: tcex42a.POLY3
 CPU time for mapping          11  seconds
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-lab e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-text x n MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-title example 42a
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST:
POST: make tcex42 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
POST: back
POLY_3: read tcex42a
   ... the command in full is READ_WORKSPACES
POLY_3: s-a-v 1 t 800 1200 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex42b y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  para
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/:  C
Fast diffusing component: /NONE/:
 Output during stepping is:
```

```
 axis value, phase amounts, u-fractions of interstitial(s) in    phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824   4.977501E-02   6.609390E-04  -2.303643E-01
   8.900000E+02    0.161    0.839   5.421135E-02   6.889794E-04  -1.689777E-02
   8.800000E+02    0.148    0.852   5.872152E-02   7.140931E-04   1.943989E-01
   8.700000E+02    0.137    0.863   6.329608E-02   7.362105E-04   4.040959E-01
   8.600000E+02    0.127    0.873   6.792661E-02   7.552871E-04   6.126989E-01
   8.500000E+02    0.119    0.881   7.260558E-02   7.713010E-04   8.206607E-01
   8.400000E+02    0.111    0.889   7.732629E-02   7.842505E-04   1.028392E+00
   8.300000E+02    0.105    0.895   8.208278E-02   7.941530E-04   1.236267E+00
   8.200000E+02    0.099    0.901   8.686971E-02   8.010431E-04   1.444633E+00
   8.100000E+02    0.093    0.907   9.168236E-02   8.049714E-04   1.653814E+00
   8.000000E+02    0.089    0.911   9.651648E-02   8.060032E-04   1.864114E+00

 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824   4.977501E-02   6.609390E-04  -2.303643E-01
   9.100000E+02    0.193    0.807   4.542308E-02   6.300692E-04  -4.466511E-01
   9.200000E+02    0.214    0.786   4.116735E-02   5.964982E-04  -6.665081E-01
   9.300000E+02    0.240    0.760   3.702095E-02   5.603899E-04  -8.908100E-01
   9.400000E+02    0.270    0.730   3.299845E-02   5.219482E-04  -1.120589E+00
   9.500000E+02    0.308    0.692   2.911596E-02   4.814238E-04  -1.357076E+00
   9.600000E+02    0.355    0.645   2.539121E-02   4.391211E-04  -1.601760E+00
   9.700000E+02    0.415    0.585   2.184354E-02   3.954079E-04  -1.856463E+00
   9.800000E+02    0.493    0.507   1.849394E-02   3.507265E-04  -2.123436E+00
   9.900000E+02    0.597    0.403   1.536496E-02   3.056079E-04  -2.405499E+00
   1.000000E+03    0.739    0.261   1.248054E-02   2.606888E-04  -2.706208E+00
   1.010000E+03    0.942    0.058   9.852896E-03   2.164281E-04  -3.031479E+00
   1.020000E+03    1.259   -0.259   7.420594E-03   1.715531E-04  -3.400603E+00
   1.030000E+03    1.821   -0.821   5.161354E-03   1.256551E-04  -3.846325E+00
   1.040000E+03    3.087   -2.087   3.063915E-03   7.858616E-05  -4.447717E+00
   1.050000E+03    8.516   -7.516   1.118169E-03   3.022614E-05  -5.532996E+00
 *** Buffer savend on file tcex42b.POLY3

 *** ERROR     8 IN NS01AD
 *** Numerical error
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 42b
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST:
POST: ap-e y tcex42
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  1
POST: s-s x n 0 0.02
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 800 1200
   ... the command in full is SET_SCALING_STATUS
POST: set-tit example 42c
   ... the command in full is SET_TITLE
POST: plot
```

```
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:@?
POST:
POST: back
POLY_3: read tcex42b
   ... the command in full is READ_WORKSPACES
POLY_3: s-c w(c)=0.01
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        11623  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=900, P=1E5, N=1, W(C)=1E-2, W(MN)=2.5E-2
 DEGREES OF FREEDOM 0

 Temperature    900.00 K (   626.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.38780E+01
 Total Gibbs energy -3.55135E+04,  Enthalpy  2.04087E+04,  Volume  7.05542E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.4413E-02  1.0000E-02 2.8953E-01 -9.2753E+03 SER
 FE                      9.3131E-01  9.7500E-01 8.2548E-03 -3.5896E+04 SER
 MN                      2.4275E-02  2.5000E-02 1.0105E-04 -6.8844E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 8.2304E-01, Mass 4.5951E+01, Volume fraction 8.4974E-01  Mass fractions:
 FE  9.92487E-01  MN  7.46758E-03  C   4.52842E-05

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.7696E-01, Mass 7.9270E+00, Volume fraction 1.5026E-01  Mass fractions:
 FE  8.08018E-01  MN  1.24950E-01  C   6.70326E-02
POLY_3:
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  para
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: cem
Fast diffusing component: /C/:  C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in    phase 1 and 2,
 and LNACR value(s) of interstitial(s)

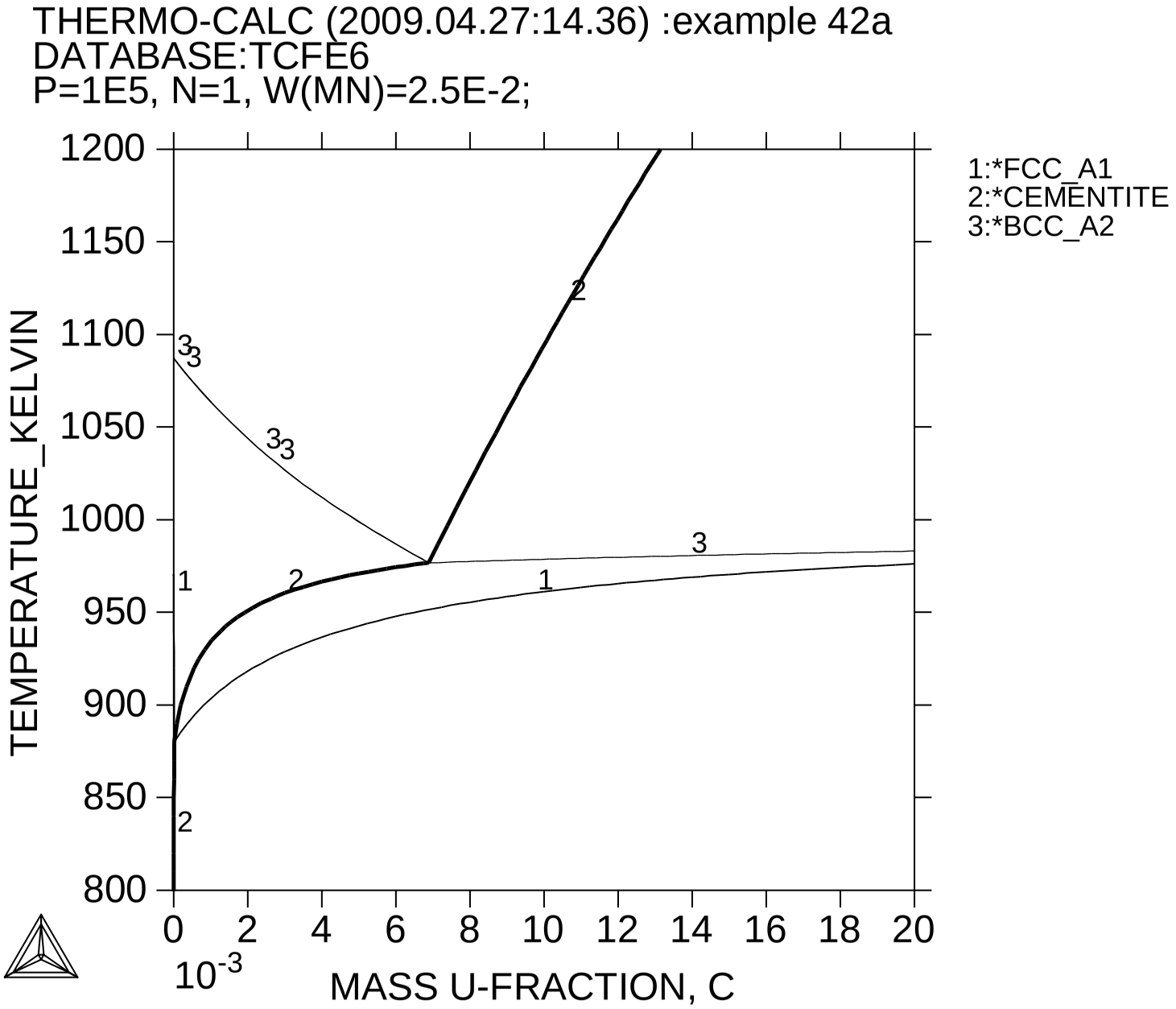
 Phase Region from    900.000     for:
     CEMENTITE
     FCC_A1
   9.000000E+02    0.932    0.068   2.554923E-02   3.333333E-01  -1.148376E+00
   8.900000E+02    0.929    0.071   2.453374E-02   3.333333E-01  -1.120519E+00
   8.800000E+02    0.926    0.074   2.353422E-02   3.333333E-01  -1.092268E+00
   8.700000E+02    0.923    0.077   2.255097E-02   3.333333E-01  -1.063621E+00
   8.600000E+02    0.920    0.080   2.158434E-02   3.333333E-01  -1.034574E+00
   8.500000E+02    0.917    0.083   2.063468E-02   3.333333E-01  -1.005126E+00
   8.400000E+02    0.915    0.085   1.970236E-02   3.333333E-01  -9.752721E-01
   8.300000E+02    0.912    0.088   1.878777E-02   3.333333E-01  -9.450113E-01
   8.200000E+02    0.909    0.091   1.789129E-02   3.333333E-01  -9.143405E-01
   8.100000E+02    0.907    0.093   1.701335E-02   3.333333E-01  -8.832577E-01
   8.000000E+02    0.904    0.096   1.615437E-02   3.333333E-01  -8.517606E-01

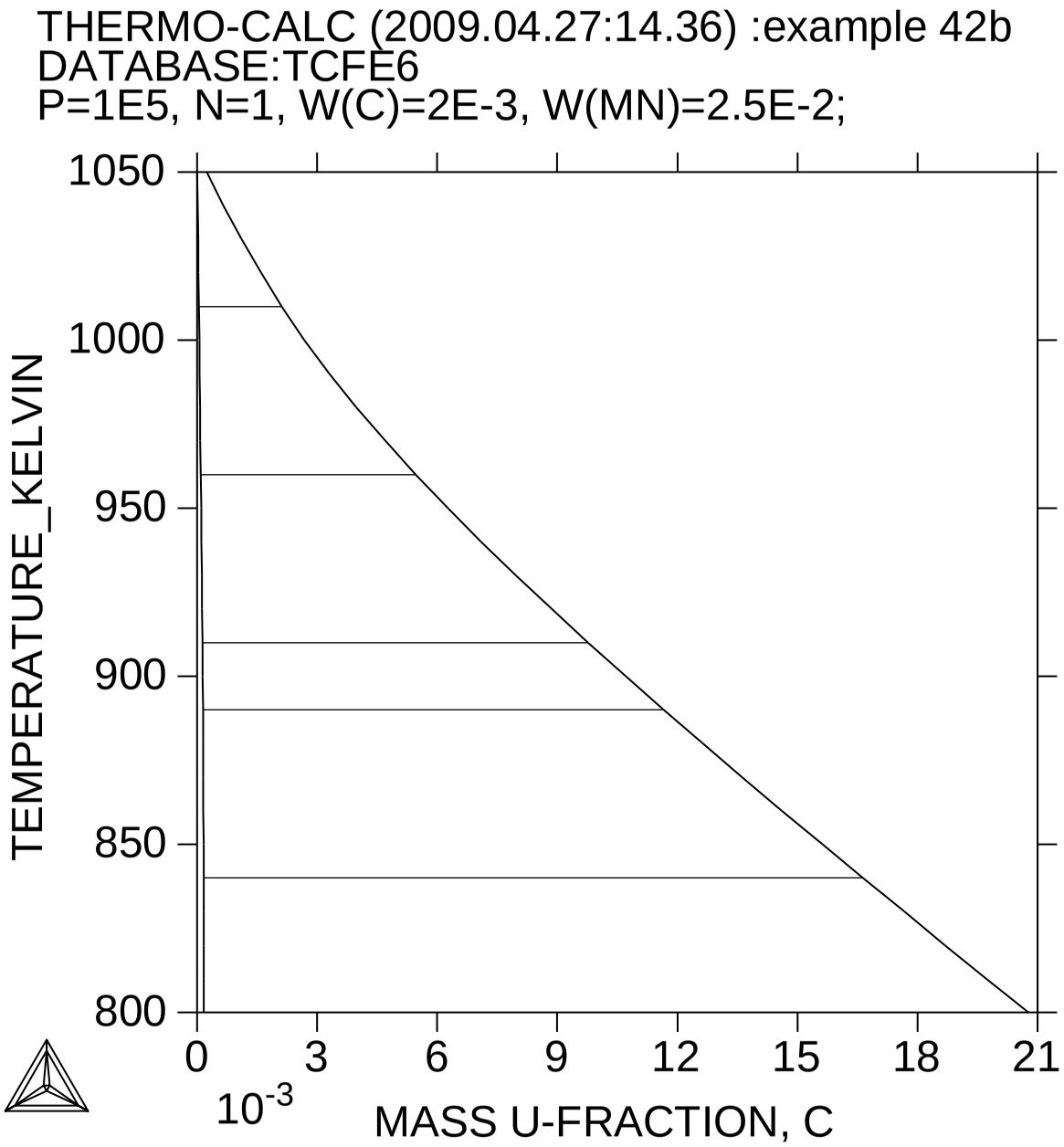
 Phase Region from    900.000     for:
     CEMENTITE
     FCC_A1
   9.000000E+02    0.932    0.068   2.554923E-02   3.333333E-01  -1.148376E+00
```

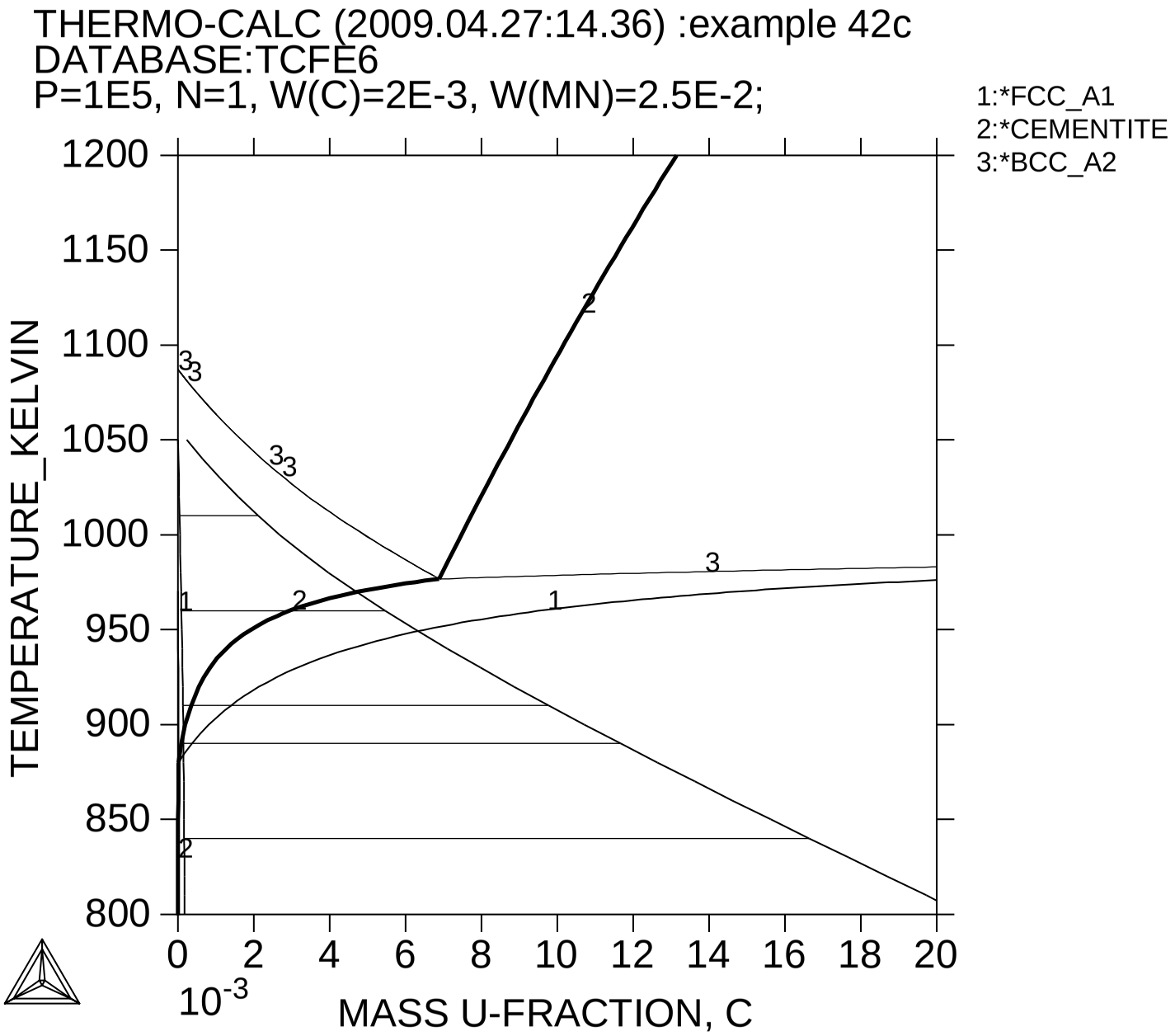
```
   9.100000E+02    0.935    0.065   2.658037E-02   3.333333E-01  -1.175842E+00
   9.200000E+02    0.938    0.062   2.762688E-02   3.333333E-01  -1.202921E+00
   9.300000E+02    0.942    0.058   2.868849E-02   3.333333E-01  -1.229615E+00
   9.400000E+02    0.945    0.055   2.976496E-02   3.333333E-01  -1.255928E+00
   9.500000E+02    0.948    0.052   3.085606E-02   3.333333E-01  -1.281861E+00
   9.600000E+02    0.952    0.048   3.196156E-02   3.333333E-01  -1.307420E+00
   9.700000E+02    0.955    0.045   3.308128E-02   3.333333E-01  -1.332605E+00
   9.800000E+02    0.959    0.041   3.421503E-02   3.333333E-01  -1.357420E+00
   9.900000E+02    0.963    0.037   3.536265E-02   3.333333E-01  -1.381869E+00
   1.000000E+03    0.966    0.034   3.652401E-02   3.333333E-01  -1.405953E+00
   1.010000E+03    0.970    0.030   3.769896E-02   3.333333E-01  -1.429677E+00
   1.020000E+03    0.974    0.026   3.888741E-02   3.333333E-01  -1.453041E+00
   1.030000E+03    0.978    0.022   4.008925E-02   3.333333E-01  -1.476050E+00
   1.040000E+03    0.982    0.018   4.130440E-02   3.333333E-01  -1.498705E+00
   1.050000E+03    0.986    0.014   4.253282E-02   3.333333E-01  -1.521010E+00
   1.060000E+03    0.991    0.009   4.377444E-02   3.333333E-01  -1.542967E+00
   1.070000E+03    0.995    0.005   4.502924E-02   3.333333E-01  -1.564577E+00
   1.080000E+03    0.999    0.001   4.629720E-02   3.333333E-01  -1.585844E+00
   1.090000E+03    1.004   -0.004   4.757831E-02   3.333333E-01  -1.606770E+00
   1.100000E+03    1.008   -0.008   4.887260E-02   3.333333E-01  -1.627357E+00
   1.110000E+03    1.013   -0.013   5.018009E-02   3.333333E-01  -1.647607E+00
   1.120000E+03    1.018   -0.018   5.150082E-02   3.333333E-01  -1.667522E+00
   1.130000E+03    1.023   -0.023   5.283486E-02   3.333333E-01  -1.687104E+00
   1.140000E+03    1.028   -0.028   5.418227E-02   3.333333E-01  -1.706354E+00
   1.150000E+03    1.033   -0.033   5.554314E-02   3.333333E-01  -1.725275E+00
   1.160000E+03    1.038   -0.038   5.691756E-02   3.333333E-01  -1.743868E+00
   1.170000E+03    1.043   -0.043   5.830566E-02   3.333333E-01  -1.762134E+00
   1.180000E+03    1.048   -0.048   5.970756E-02   3.333333E-01  -1.780075E+00
   1.190000E+03    1.054   -0.054   6.112340E-02   3.333333E-01  -1.797692E+00
   1.200000E+03    1.059   -0.059   6.255334E-02   3.333333E-01  -1.814987E+00
 *** Buffer savend on file tcex42b.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

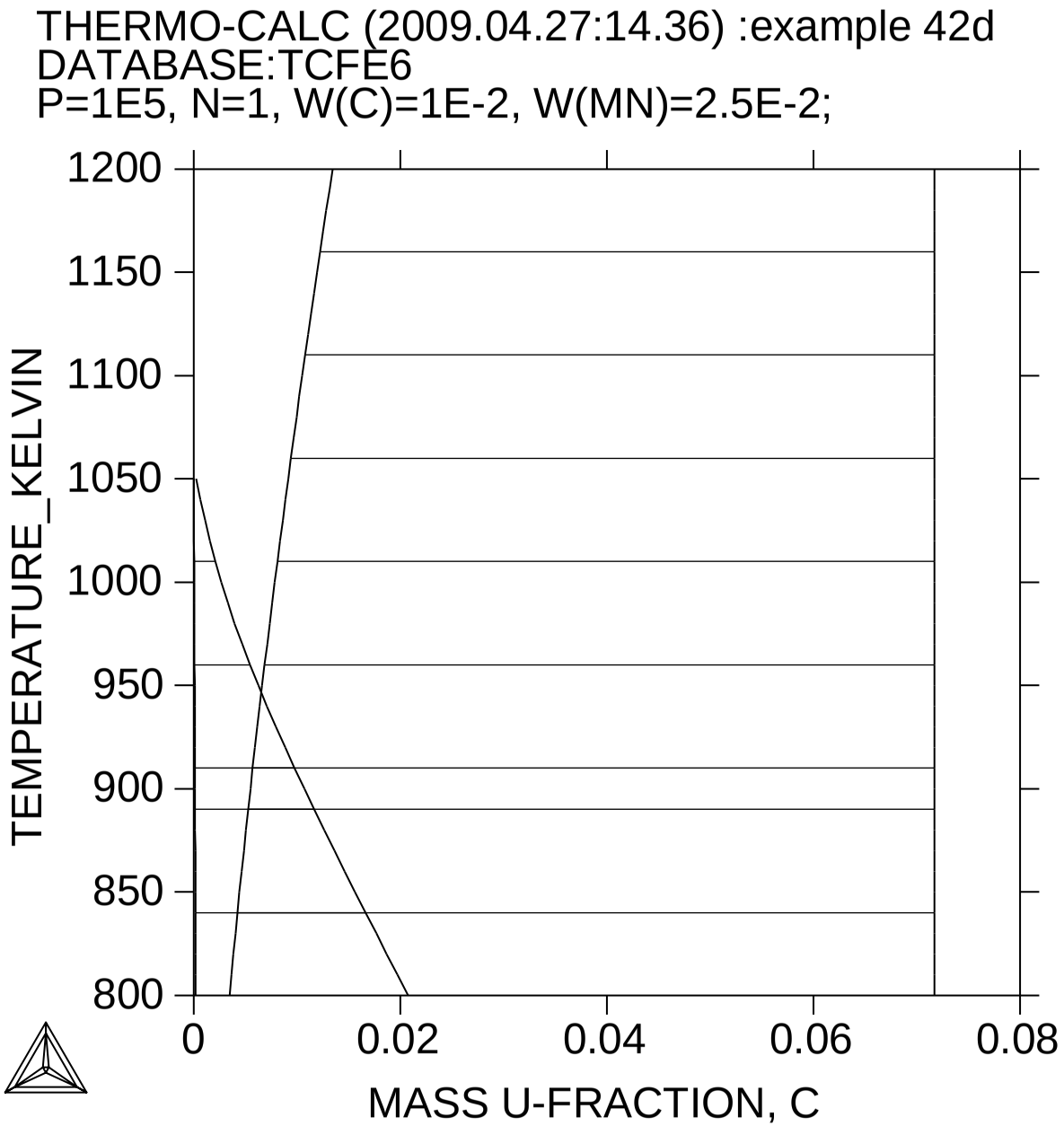
 Setting automatic diagram axis

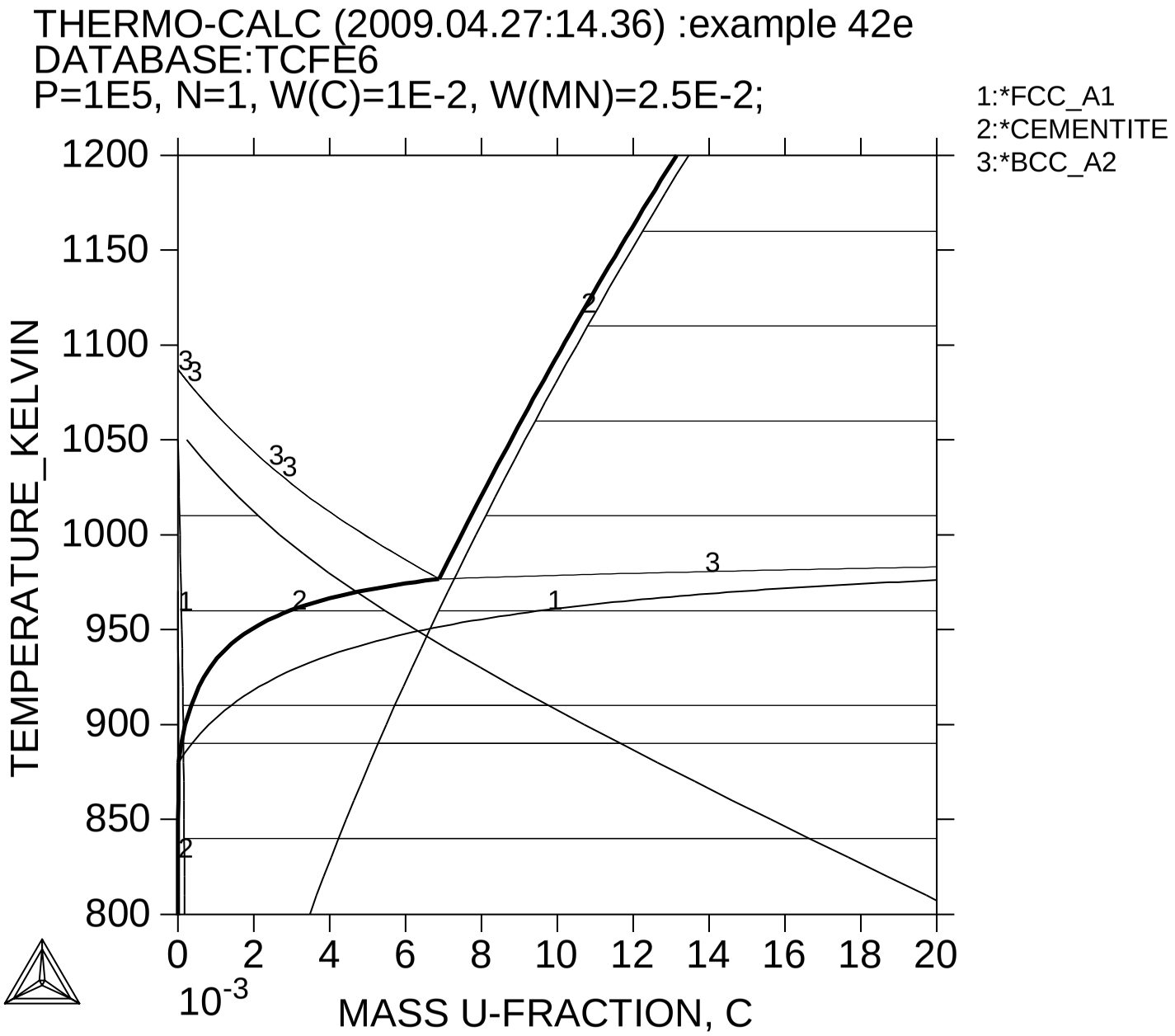
POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-tit example 42d
   ... the command in full is SET_TITLE
POST: app-e n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST:
POST: app-e y tcex42
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
DATASET NUMBER(s): /-1/:  1
POST: s-s x n 0 0.02
   ... the command in full is SET_SCALING_STATUS
POST: set-tit example 42e
   ... the command in full is SET_TITLE
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time          18  seconds
```


THERMO-CALC (2009.04.27:14.36) :example 42a
DATABASE:TCFE6
P=1E5, N=1, W(MN)=2.5E-2;
1200
1150
1100
1050
1000
950
900
850
800
TEMPERATURE_KELVIN
0
2
4
6
8
10
12
14
16
18
20
10-3
MASS U-FRACTION, C
1:*FCC_A1
2:*CEMENTITE
3:*BCC_A2


THERMO-CALC (2009.04.27:14.36) :example 42b
DATABASE:TCFE6
P=1E5, N=1, W(C)=2E-3, W(MN)=2.5E-2;
1050
1000
950
900
850
800
TEMPERATURE_KELVIN
0
3
6
9
12
15
18
21
10-3
MASS U-FRACTION, C


THERMO-CALC (2009.04.27:14.36) :example 42c
DATABASE:TCFE6
P=1E5, N=1, W(C)=2E-3, W(MN)=2.5E-2;
1:*FCC_A1
2:*CEMENTITE
3:*BCC_A2
TEMPERATURE_KELVIN
1200
1150
1100
1050
1000
950
900
850
800
0
2
4
6
8
10
12
14
16
18
20
10-3
MASS U-FRACTION, C


THERMO-CALC (2009.04.27:14.36) :example 42d
DATABASE:TCFE6
P=1E5, N=1, W(C)=1E-2, W(MN)=2.5E-2;
1200
1150
1100
1050
1000
950
900
850
800
TEMPERATURE_KELVIN
0
0.02
0.04
0.06
0.08
MASS U-FRACTION, C


THERMO-CALC (2009.04.27:14.36) :example 42e
DATABASE:TCFE6
P=1E5, N=1, W(C)=1E-2, W(MN)=2.5E-2;
1:*FCC_A1
2:*CEMENTITE
3:*BCC_A2
TEMPERATURE_KELVIN
1200
1150
1100
1050
1000
950
900
850
800
0
2
4
6
8
10
12
14
16
18
20
10-3
MASS U-FRACTION, C

43

Formation of Para-pearlite (Calculation of Isothermal Section)

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Paraequilibrium calculation - Formation of Para-pearlite - Isothermal
SYS: @@
SYS: @@  Fe-Mn-C system at 700 C
SYS: @@
SYS: set-log ex43,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: d-mater
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/:  tcfe6
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:  Y
1st alloying element: c 0.1
2nd alloying element: mn 2
Next alloying element:
Temperature (C) /1000/:  700
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED

 This database has following phases for the defined system

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    KSI_CARBIDE             A1_KAPPA
 KAPPA                   FE4N_LP1                FECN_CHI
 LAVES_PHASE_C14

Reject phase(s) /NONE/:  graphite m5c2
 GRAPHITE                M5C2  REJECTED
Reject phase(s) /NONE/:  NONE
Restore phase(s): /NONE/:  NONE
 ..................................................

    The following phases are retained in this system:

 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          CEMENTITE
 M23C6                   M7C3                    KSI_CARBIDE
 A1_KAPPA                KAPPA                   FE4N_LP1
 FECN_CHI                LAVES_PHASE_C14

 ..................................................

OK? /Y/:  Y
 ELEMENTS .....
 SPECIES ......
```

```
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'P. Franke, estimated parameter within SGTE, 2008; Fe-Mn-C'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
                    :
                    :
                    :
  'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C-FE-MO'
  'D. Connetable, J. Lacaze, P. Maugis and B. Sundman; Accepted in CALPHAD,
      2008; Al-C-Fe'
  'Thermo-Calc Software (2008): Volume data updated for TCFE6 database (TCFE
      v6, April, 2008).'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'Estimated parameter for solubility of C in Fe4N, 1999'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
 -OK-
Should any phase have a miscibility gap check? /N/:  N
 Using global minimization procedure
 Calculated        11623  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=973.15, W(C)=1E-3, W(MN)=2E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    973.15 K (   700.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.56256E+01
 Total Gibbs energy -4.11739E+04,  Enthalpy  2.46047E+04,  Volume  7.28123E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.6312E-03  1.0000E-03 1.2824E-01 -1.6618E+04 SER
 FE                      9.7512E-01  9.7900E-01 6.6199E-03 -4.0599E+04 SER
 MN                      2.0250E-02  2.0000E-02 1.0082E-04 -7.4457E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.8346E-01, Mass 4.3734E+01, Volume fraction 7.8722E-01  Mass fractions:
 FE  9.86998E-01  MN  1.29345E-02  C   6.74179E-05

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 2.1654E-01, Mass 1.1892E+01, Volume fraction 2.1278E-01  Mass fractions:
 FE  9.49585E-01  MN  4.59849E-02  C   4.42980E-03
POLY_3: @@
POLY_3: @@ change the status of component C to SPECIAL and work with u-fractions
POLY_3: @@
POLY_3: c-s comp c
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:  spe
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        11623  grid points in            0  s
```

```
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 w(c) 0 0.08
   ... the command in full is SET_AXIS_VARIABLE
Increment /.002/:  2.5E-04
POLY_3: s-a-v 2 w(mn) 0 0.1
   ... the command in full is SET_AXIS_VARIABLE
Increment /.0025/:  .0025
POLY_3: l-a-v
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(C)                 Min: 0         Max: 8E-2      Inc: 2.5E-4
  Axis No 2: W(MN)                Min: 0         Max: 0.1       Inc: 2.5E-3
POLY_3: sa tcex43a y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
 Generating start point  31
 Generating start point  32

 Phase region boundary   1 at:   3.082E-02  1.466E-02
     BCC_A2
  ** CEMENTITE
 *** Buffer saved on file: tcex43a.POLY3
 Calculated           18  equilibria
```

```
 Phase region boundary   2 at:   3.082E-02  1.466E-02
     BCC_A2
  ** CEMENTITE
 Calculated.           11  equilibria

 Phase region boundary   3 at:   3.082E-02  3.943E-02
     BCC_A2
  ** CEMENTITE
  ** FCC_A1

 Phase region boundary   4 at:   3.392E-03  1.781E-02
     BCC_A2
  ** FCC_A1
 Calculated           34  equilibria

       :
       :
       :

 Phase region boundary  40 at:   3.590E-01  9.750E-02
     CEMENTITE
  ** DIAMOND_FCC_A4
 Calculated           42  equilibria

 Phase region boundary  41 at:   3.590E-01  9.750E-02
     CEMENTITE
  ** DIAMOND_FCC_A4
 Calculated.           95  equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   3.590E-01  9.750E-02
     CEMENTITE
  ** DIAMOND_FCC_A4
 Calculated           42  equilibria

 Phase region boundary  43 at:   3.590E-01  9.750E-02
     CEMENTITE
  ** DIAMOND_FCC_A4
 Calculated.           95  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex43a.POLY3
 CPU time for mapping          10  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-lab e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 43a
POST: s-ax-text x N MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N MASS U-FRACTION, MN
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST:
POST: make tcex43 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: b
   ... the command in full is BACK
POLY_3: read tcex43a
   ... the command in full is READ_WORKSPACES
POLY_3: s-a-v 1 w(mn) 0 0.1
   ... the command in full is SET_AXIS_VARIABLE
Increment /.0025/:  .0025
POLY_3: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex43b y
```

```
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  para
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/:  C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in    phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from   0.200000E-01 for:
     BCC_A2
     FCC_A1
   2.000000E-02    0.165    0.835   2.571485E-02   4.910396E-04  -1.652126E+00
   1.750000E-02    0.148    0.852   2.818000E-02   5.485823E-04  -1.524121E+00
   1.500000E-02    0.135    0.865   3.063880E-02   6.079802E-04  -1.404111E+00
   1.250000E-02    0.123    0.877   3.309067E-02   6.692476E-04  -1.290883E+00
   1.000000E-02    0.113    0.887   3.553566E-02   7.324129E-04  -1.183465E+00
   7.500000E-03    0.104    0.896   3.797362E-02   7.974991E-04  -1.081091E+00
   5.000000E-03    0.096    0.904   4.040445E-02   8.645295E-04  -9.831360E-01
   2.500000E-03    0.089    0.911   4.282805E-02   9.335273E-04  -8.890905E-01
   2.500000E-09    0.082    0.918   4.524437E-02   1.004515E-03  -7.985285E-01

 Phase Region from   0.200000E-01 for:
     BCC_A2
     FCC_A1
   2.000000E-02    0.165    0.835   2.571485E-02   4.910396E-04  -1.652126E+00
   2.250000E-02    0.185    0.815   2.324342E-02   4.353248E-04  -1.789740E+00
   2.500000E-02    0.209    0.791   2.076601E-02   3.814145E-04  -1.939115E+00
   2.750000E-02    0.241    0.759   1.828295E-02   3.292857E-04  -2.103233E+00
   3.000000E-02    0.282    0.718   1.579466E-02   2.789151E-04  -2.286396E+00
   3.250000E-02    0.338    0.662   1.330158E-02   2.302795E-04  -2.495141E+00
   3.500000E-02    0.420    0.580   1.080428E-02   1.833559E-04  -2.740125E+00
   3.750000E-02    0.552    0.448   8.303377E-03   1.381213E-04  -3.040528E+00
   4.000000E-02    0.798    0.202   5.799614E-03   9.455272E-05  -3.436595E+00
   4.250000E-02    1.418   -0.418   3.293836E-03   5.262739E-05  -4.039594E+00
   4.500000E-02    5.984   -4.984   7.870255E-04   1.232263E-05  -5.508458E+00
 *** Buffer savend on file tcex43b.POLY3

 *** ERROR     3 IN NS01AD
 *** Numerical error
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: s-d-a y w(*,mn)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 43b
POST: s-ax-text x N MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N MASS U-FRACTION, MN
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST:
POST: app y tcex43
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/:  0
```

```
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.01
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.08
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 43c
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST:
POST: b
   ... the command in full is BACK
POLY_3: read tcex43b
   ... the command in full is READ_WORKSPACES
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=973.15, W(C)=1E-3, W(MN)=2E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY_3: s-c w(c)=0.008 w(mn)=0.07
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated        11623  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 T=973.15, W(C)=8E-3, W(MN)=7E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    973.15 K (   700.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.42144E+01
 Total Gibbs energy -4.19857E+04,  Enthalpy  2.75863E+04,  Volume  7.10872E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.5823E-02  8.0000E-03 1.8345E-01 -1.3721E+04 SER
 FE                      8.9565E-01  9.3000E-01 6.4227E-03 -4.0844E+04 SER
 MN                      6.8530E-02  7.0000E-02 1.4208E-04 -7.1681E+04 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.7022E-01, Mass 5.2881E+01, Volume fraction 9.7477E-01  Mass fractions:
 FE  9.26648E-01  MN  6.69068E-02  C   6.44559E-03

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.9780E-02, Mass 1.3330E+00, Volume fraction 2.5229E-02  Mass fractions:
 FE  7.62802E-01  MN  1.70116E-01  C   6.70826E-02
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: cem
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 NP(FCC) =   0.9928 with U-fractions C  =  3.50068E-02
 NP(CEM) =   0.0072 with U-fractions C  =  3.33333E-01
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: cem
```

```
Fast diffusing component: /C/:  C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in    phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from   0.700000E-01 for:
     CEMENTITE
     FCC_A1
   7.000000E-02    0.993    0.007   3.500676E-02   3.333333E-01  -1.512238E+00
   6.750000E-02    0.993    0.007   3.491610E-02   3.333333E-01  -1.502576E+00
   6.500000E-02    0.992    0.008   3.482586E-02   3.333333E-01  -1.492928E+00
   6.250000E-02    0.992    0.008   3.473603E-02   3.333333E-01  -1.483293E+00
   6.000000E-02    0.992    0.008   3.464662E-02   3.333333E-01  -1.473672E+00
   5.750000E-02    0.991    0.009   3.455761E-02   3.333333E-01  -1.464066E+00
   5.500000E-02    0.991    0.009   3.446901E-02   3.333333E-01  -1.454473E+00
   5.250000E-02    0.991    0.009   3.438081E-02   3.333333E-01  -1.444894E+00
   5.000000E-02    0.990    0.010   3.429302E-02   3.333333E-01  -1.435329E+00
   4.750000E-02    0.990    0.010   3.420563E-02   3.333333E-01  -1.425778E+00
   4.500000E-02    0.990    0.010   3.411864E-02   3.333333E-01  -1.416242E+00
   4.250000E-02    0.990    0.010   3.403205E-02   3.333333E-01  -1.406719E+00
   4.000000E-02    0.989    0.011   3.394585E-02   3.333333E-01  -1.397211E+00
   3.750000E-02    0.989    0.011   3.386005E-02   3.333333E-01  -1.387717E+00
   3.500000E-02    0.989    0.011   3.377464E-02   3.333333E-01  -1.378237E+00
   3.250000E-02    0.988    0.012   3.368963E-02   3.333333E-01  -1.368772E+00
   3.000000E-02    0.988    0.012   3.360500E-02   3.333333E-01  -1.359321E+00
   2.750000E-02    0.988    0.012   3.352076E-02   3.333333E-01  -1.349884E+00
   2.500000E-02    0.988    0.012   3.343690E-02   3.333333E-01  -1.340462E+00
   2.250000E-02    0.987    0.013   3.335343E-02   3.333333E-01  -1.331054E+00
   2.000000E-02    0.987    0.013   3.327034E-02   3.333333E-01  -1.321660E+00
   1.750000E-02    0.987    0.013   3.318763E-02   3.333333E-01  -1.312282E+00
   1.500000E-02    0.987    0.013   3.310530E-02   3.333333E-01  -1.302918E+00
   1.250000E-02    0.986    0.014   3.302335E-02   3.333333E-01  -1.293568E+00
   1.000000E-02    0.986    0.014   3.294177E-02   3.333333E-01  -1.284233E+00
   7.500000E-03    0.986    0.014   3.286057E-02   3.333333E-01  -1.274913E+00
   5.000000E-03    0.985    0.015   3.277974E-02   3.333333E-01  -1.265607E+00
   2.500000E-03    0.985    0.015   3.269928E-02   3.333333E-01  -1.256316E+00
   2.500000E-09    0.985    0.015   3.261919E-02   3.333333E-01  -1.247040E+00

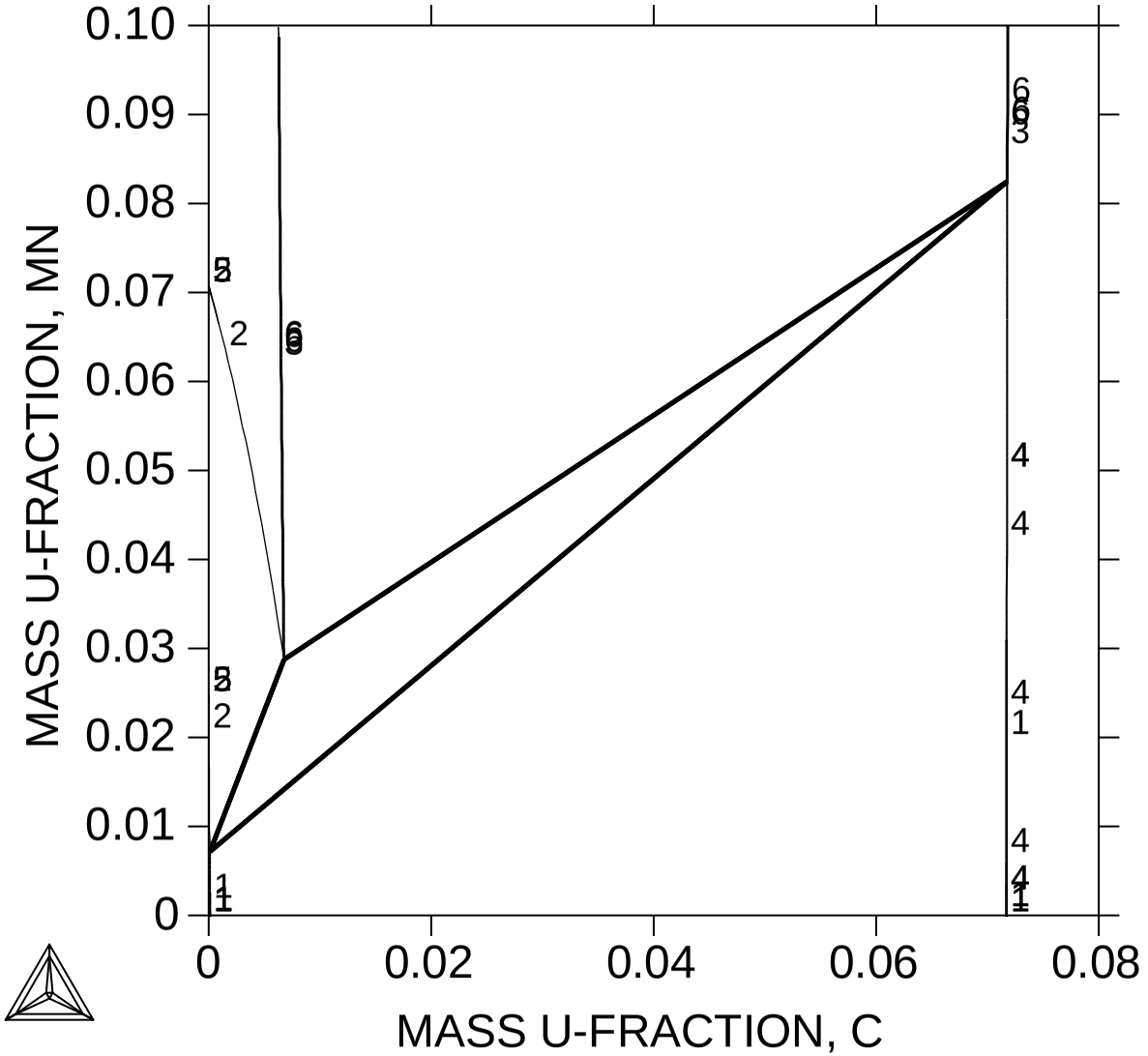
 Phase Region from   0.700000E-01 for:
     CEMENTITE
     FCC_A1
   7.000000E-02    0.993    0.007   3.500676E-02   3.333333E-01  -1.512238E+00
   7.250000E-02    0.993    0.007   3.509783E-02   3.333333E-01  -1.521914E+00
   7.500000E-02    0.993    0.007   3.518931E-02   3.333333E-01  -1.531604E+00
   7.750000E-02    0.994    0.006   3.528122E-02   3.333333E-01  -1.541307E+00
   8.000000E-02    0.994    0.006   3.537355E-02   3.333333E-01  -1.551024E+00
   8.250000E-02    0.994    0.006   3.546630E-02   3.333333E-01  -1.560755E+00
   8.500000E-02    0.995    0.005   3.555948E-02   3.333333E-01  -1.570499E+00
   8.750000E-02    0.995    0.005   3.565309E-02   3.333333E-01  -1.580257E+00
   9.000000E-02    0.995    0.005   3.574712E-02   3.333333E-01  -1.590028E+00
   9.250000E-02    0.996    0.004   3.584159E-02   3.333333E-01  -1.599812E+00
   9.500000E-02    0.996    0.004   3.593649E-02   3.333333E-01  -1.609610E+00
   9.750000E-02    0.996    0.004   3.603182E-02   3.333333E-01  -1.619421E+00
   1.000000E-01    0.997    0.003   3.612760E-02   3.333333E-01  -1.629246E+00
 *** Buffer savend on file tcex43b.POLY3
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: s-d-a y w(*,mn)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:  *
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 43d
POST: s-ax-text x N MASS U-FRACTION, C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N MASS U-FRACTION, MN
   ... the command in full is SET_AXIS_TEXT_STATUS
```

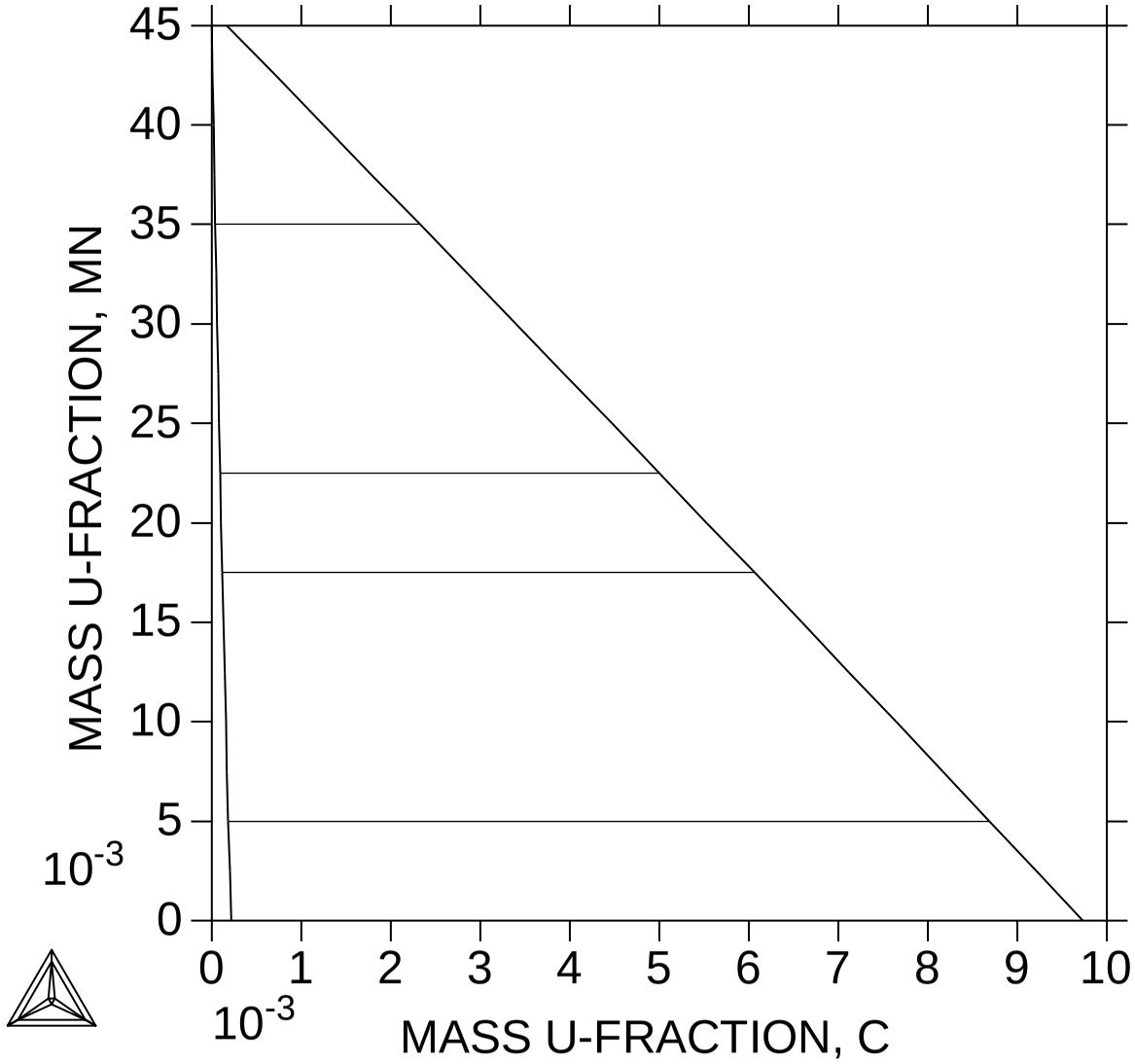
POST: **app-e n**
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: **pl**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST:**@?**
POST:
POST: **s-s x n 0 0.01**
   ... the command in full is SET_SCALING_STATUS
POST: **s-s y n 0 0.10**
   ... the command in full is SET_SCALING_STATUS
POST: **app-e y tcex43**
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: **0**
DATASET NUMBER(s): /-1/: **1**
POST: **set-title example 43e**
POST: **pl**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: **set-inter**
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time   17 seconds

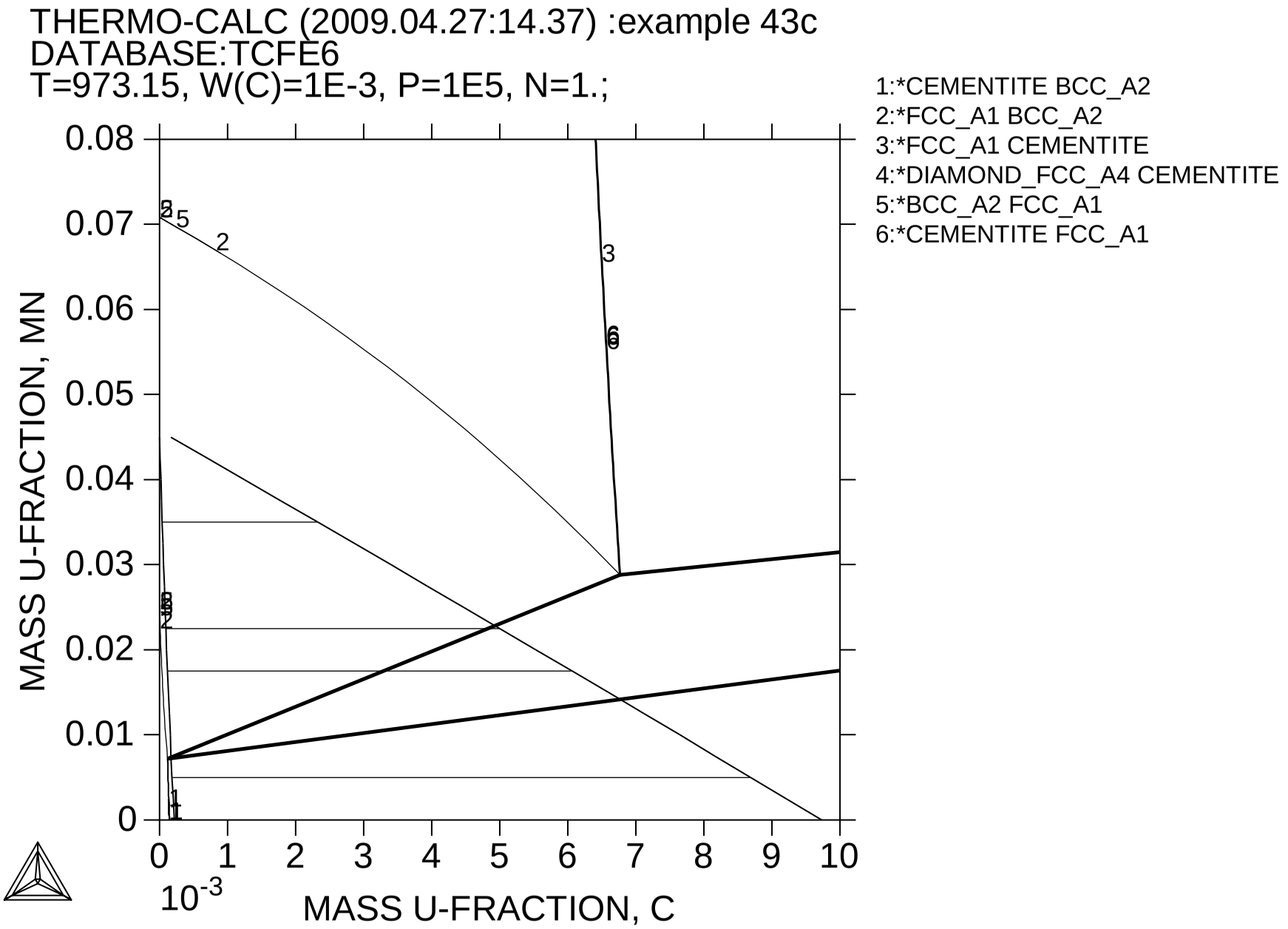
THERMO-CALC (2009.04.27:14.37) :example 43a
DATABASE:TCFE6
T=973.15, P=1E5, N=1;

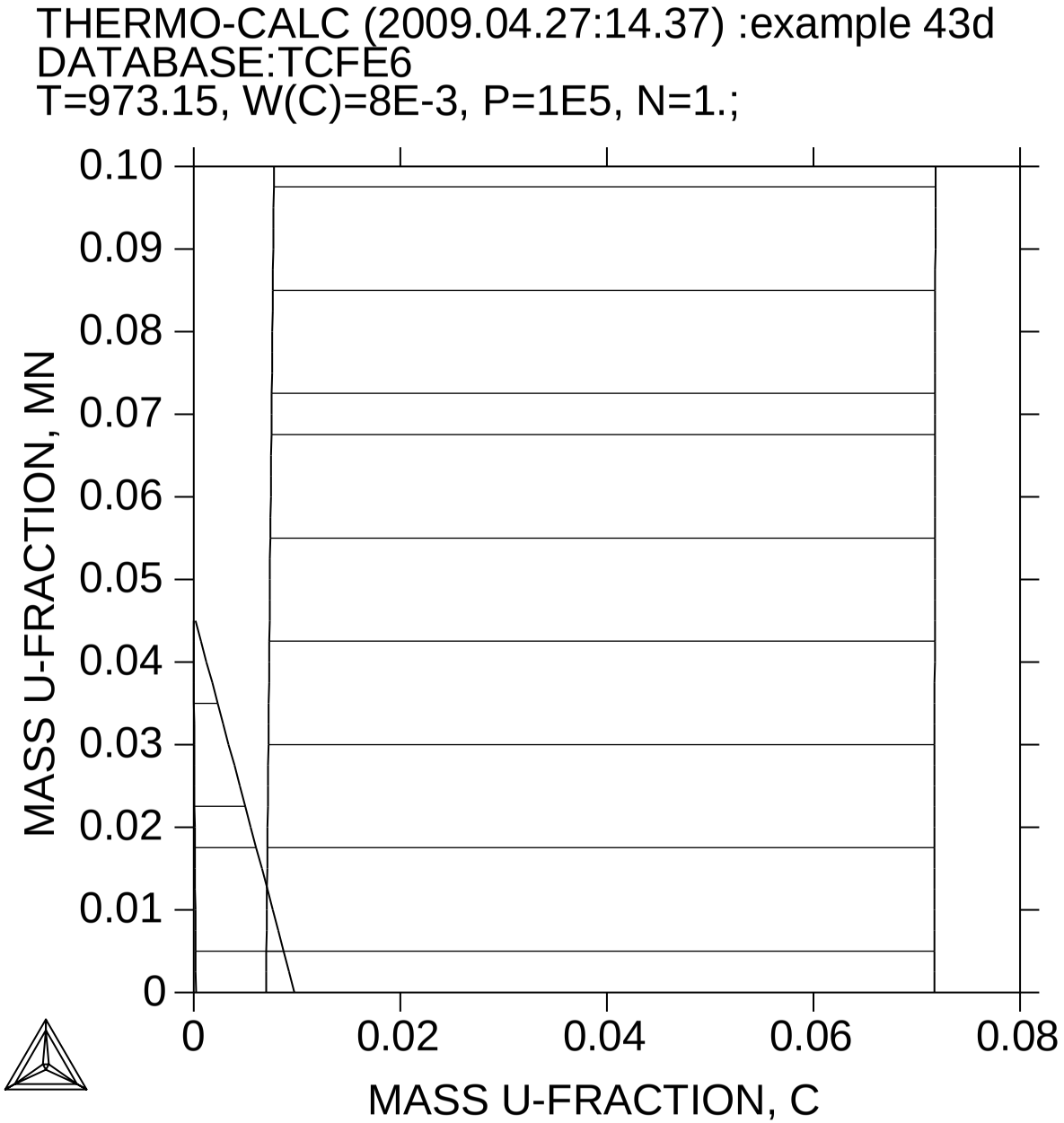


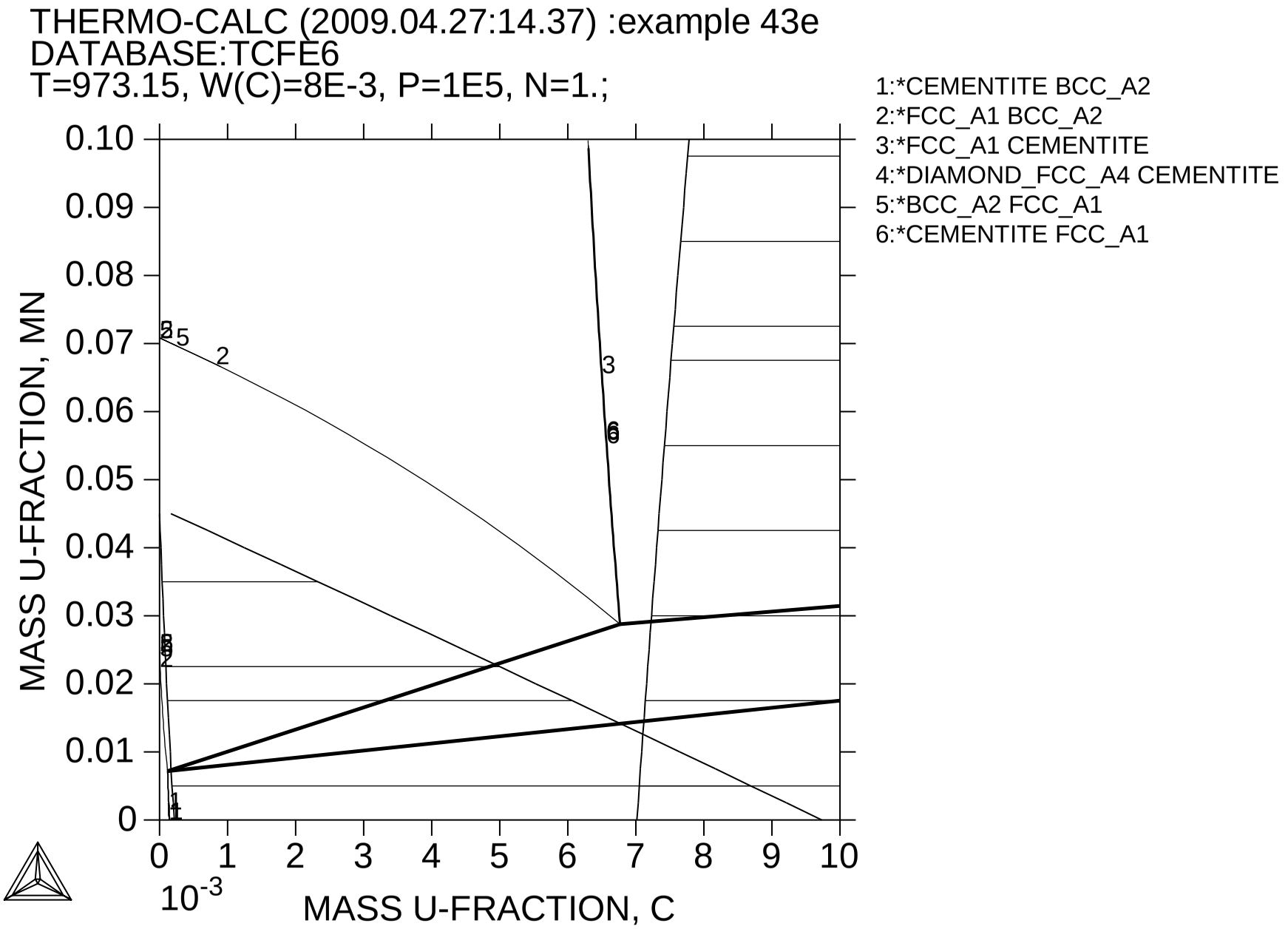
1:*CEMENTITE BCC_A2
2:*FCC_A1 BCC_A2
3:*FCC_A1 CEMENTITE
4:*DIAMOND_FCC_A4 CEMENTITE
5:*BCC_A2 FCC_A1
6:*CEMENTITE FCC_A1

THERMO-CALC (2009.04.27:14.37) :example 43b
DATABASE:TCFE6
T=973.15, W(C)=1E-3, P=1E5, N=1.;




THERMO-CALC (2009.04.27:14.37) :example 43c
DATABASE:TCFE6
T=973.15, W(C)=1E-3, P=1E5, N=1.;
1:*CEMENTITE BCC_A2
2:*FCC_A1 BCC_A2
3:*FCC_A1 CEMENTITE
4:*DIAMOND_FCC_A4 CEMENTITE
5:*BCC_A2 FCC_A1
6:*CEMENTITE FCC_A1
MASS U-FRACTION, MN
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0 1 2 3 4 5 6 7 8 9 10
10-3
MASS U-FRACTION, C


THERMO-CALC (2009.04.27:14.37) :example 43d
DATABASE:TCFE6
T=973.15, W(C)=8E-3, P=1E5, N=1.;
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
MASS U-FRACTION, MN
0
0.02
0.04
0.06
0.08
MASS U-FRACTION, C


THERMO-CALC (2009.04.27:14.37) :example 43e
DATABASE:TCFE6
T=973.15, W(C)=8E-3, P=1E5, N=1.;
1:*CEMENTITE BCC_A2
2:*FCC_A1 BCC_A2
3:*FCC_A1 CEMENTITE
4:*DIAMOND_FCC_A4 CEMENTITE
5:*BCC_A2 FCC_A1
6:*CEMENTITE FCC_A1
MASS U-FRACTION, MN
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0 1 2 3 4 5 6 7 8 9 10
10-3
MASS U-FRACTION, C

44

Proof strength for an austenitic stainless steel at elevated temperatures

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Exploring the usage of variables and functions in order to predict
SYS: @@ properties e.g. Proof strength for an austenitic stainless
SYS: @@ steel (20-550C)
SYS:
SYS: go da
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw tcfe6
TDB_TCFE6: def-sys
ELEMENTS: fe c si mn cr ni mo cu n
 FE                      C                       SI
 MN                      CR                      NI
 MO                      CU                      N
   DEFINED
TDB_TCFE6: get
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'P. Gustafson, Inst. Met. Res. (IM-2549, 1990); C-CU-FE'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'J-O. Andersson, Calphad, 12 (1988), 1-8; TRITA 0317 (1986); C-MO'
                    :
                    :
                    :
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'N. Saunders, COST 507 Report (1998); Al-Cu'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
       441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
  'I. Ansara, unpublished work (1991); Cr-Si'
  'A. Bolcavage and U.R. Kattner, J. Phase Equil., 2, (1996); Nb-Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Halite'
 -OK-
TDB_TCFE6:
TDB_TCFE6: go p-3
 POLY version  3.32,  Dec 2007
POLY_3:
POLY_3: s-c p=1e5,n=1,t=1353
POLY_3: s-c w(c)=0.0009,w(n)=0.0007,w(cr)=.246,w(ni)=0.2,w(mn)=0.013
POLY_3: s-c w(si)=0.013,w(cu)=0.0024,w(mo)=0.003
POLY_3: l-c
 P=1E5, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
    W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
 DEGREES OF FREEDOM 0
POLY_3: c-e
 Using global minimization procedure
 Calculated        37590  grid points in           1  s
 Found the set of lowest grid points in            0  s
```

```
 Calculated POLY solution       1 s, total time     2  s
POLY_3: l-e
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 P=1E5, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
    W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
 DEGREES OF FREEDOM 0

 Temperature   1353.00 K (  1079.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.44622E+01
 Total Gibbs energy -8.11773E+04,  Enthalpy  3.59060E+04,  Volume  7.33314E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.0809E-03  9.0000E-04 1.3015E-03 -7.4744E+04 SER
 CR                      2.5767E-01  2.4600E-01 2.7776E-03 -6.6217E+04 SER
 CU                      2.0569E-03  2.4000E-03 8.2064E-05 -1.0584E+05 SER
 FE                      5.0808E-01  5.2100E-01 1.1352E-03 -7.6282E+04 SER
 MN                      1.2887E-02  1.3000E-02 6.4090E-06 -1.3452E+05 SER
 MO                      1.7030E-03  3.0000E-03 6.1894E-05 -1.0901E+05 SER
 N                       2.7217E-03  7.0000E-04 1.5572E-07 -1.7634E+05 SER
 NI                      1.8559E-01  2.0000E-01 2.2145E-04 -9.4669E+04 SER
 SI                      2.5209E-02  1.3000E-02 3.5309E-08 -1.9303E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.9414E-01, Mass 5.4199E+01, Volume fraction 9.9484E-01  Mass fractions:
 FE  5.22768E-01  SI  1.30632E-02  CU  2.41167E-03
 CR  2.43635E-01  MN  1.30395E-02  N   7.03404E-04
 NI  2.00877E-01  MO  2.86724E-03  C   6.35548E-04

 M23C6                       Status ENTERED     Driving force  0.0000E+00
 Moles 5.8631E-03, Mass 2.6353E-01, Volume fraction 5.1567E-03  Mass fractions:
 CR  7.32446E-01  MO  3.03034E-02  N   0.00000E+00
 FE  1.57407E-01  NI  1.96875E-02  CU  0.00000E+00
 C   5.52873E-02  MN  4.86874E-03  SI  0.00000E+00
POLY_3:
POLY_3: @@ Define some variables
POLY_3: enter-symb
Constant, variable, function or table? /FUNCTION/:  variable
Name: cc
Function: 100*w(fcc,c)
&
POLY_3: ent var csi=100*w(fcc,si);
POLY_3: ent var cmn=100*w(fcc,mn);
POLY_3: ent var ccr=100*w(fcc,cr);
POLY_3: ent var cni=100*w(fcc,ni);
POLY_3: ent var cmo=100*w(fcc,mo);
POLY_3: ent var ccu=100*w(fcc,cu);
POLY_3: ent var cn=100*w(fcc,n);
POLY_3: ent var cfe=100*w(fcc,fe);
POLY_3: ent var cm23=100*bpw(m23c6);
POLY_3:
POLY_3: li-sy
 DEFINED FUNCTIONS AND VARIABLES%
    CC%=100*W(FCC_A1#1,C)
    CSI%=100*W(FCC_A1#1,SI)
    CMN%=100*W(FCC_A1#1,MN)
    CCR%=100*W(FCC_A1#1,CR)
    CNI%=100*W(FCC_A1#1,NI)
    CMO%=100*W(FCC_A1#1,MO)
    CCU%=100*W(FCC_A1#1,CU)
    CN%=100*W(FCC_A1#1,N)
    CFE%=100*W(FCC_A1#1,FE)
    CM23%=100*BPW(M23C6)
POLY_3:
POLY_3: eval
Name(s): *
 CC=6.3554801E-2
 CSI=1.3063211
 CMN=1.3039537
 CCR=24.363471
 CNI=20.087675
```

```
 CMO=0.28672407
 CCU=0.24116697
 CN=7.0340367E-2
 CFE=52.276793
 CM23=0.48388543
POLY_3:
POLY_3: enter-symb
Constant, variable, function or table? /FUNCTION/:  FUNCTION
Name: tc=t-273.15;
POLY_3:
POLY_3: @@ Enter empirical parameters as function of temperature
POLY_3: ent func bc=575-0.3686*tc;
POLY_3: ent func bsi=24.76+1.129e-4*tc*tc-0.09*tc;
POLY_3: ent func bmn=-1.4-0.007*tc;
POLY_3: ent func bcr=0.3-tc*7e-4;
POLY_3: ent func bni=5.3-tc*3.3e-3;
POLY_3: ent func bmo=6-tc*3.3e-3;
POLY_3: ent func bcu=-14+0.0116*tc;
POLY_3: ent func bn=937-2.74e-6*tc*tc*tc+5.24e-3*tc*tc-3.08*tc;
POLY_3: ent func bm23=48+0.0135*tc;
POLY_3: ent func at=1.68+4.248e-6*tc*tc-4.33e-3*tc;
POLY_3:
POLY_3: li-symb *
 DEFINED FUNCTIONS AND VARIABLES%
    CC%=100*W(FCC_A1#1,C)
    CSI%=100*W(FCC_A1#1,SI)
    CMN%=100*W(FCC_A1#1,MN)
    CCR%=100*W(FCC_A1#1,CR)
    CNI%=100*W(FCC_A1#1,NI)
    CMO%=100*W(FCC_A1#1,MO)
    CCU%=100*W(FCC_A1#1,CU)
    CN%=100*W(FCC_A1#1,N)
    CFE%=100*W(FCC_A1#1,FE)
    CM23%=100*BPW(M23C6)
    TC=T-273.15
    BC=575-.3686*TC
    BSI=24.76+1.129E-04*TC*TC-.09*TC
    BMN=-1.4-.007*TC
    BCR=.3-TC*7E-04
    BNI=5.3-TC*.0033
    BMO=6-TC*.0033
    BCU=-14+.0116*TC
    BN=937-2.74E-06*TC*TC*TC+.00524*TC*TC-3.08*TC
    BM23=48+.0135*TC
    AT=1.68+4.248E-06*TC*TC-.00433*TC
POLY_3:
POLY_3: eval
Name(s): *
 CC=6.3554801E-2
 CSI=1.3063211
 CMN=1.3039537
 CCR=24.363471
 CNI=20.087675
 CMO=0.28672407
 CCU=0.24116697
 CN=7.0340367E-2
 CFE=52.276793
 CM23=0.48388543
 TC=1079.85
 BC=176.96729
 BSI=59.223483
 BMN=-8.95895
 BCR=-0.455895
 BNI=1.736495
 BMO=2.436495
 BCU=-1.47374
 BN=271.12745
 BM23=62.577975
 AT=1.9577404
POLY_3:
POLY_3: @@ Enter an empirical expression for the proof strength combining
POLY_3: @@ the variables and function parameters previuously entered.
POLY_3: ent
Constant, variable, function or table? /FUNCTION/:  FUNCTION
```

```
Name: rp1
Function: at+bc*cc+bsi*csi+bmn*cmn+bni*cni;
POLY_3:
POLY_3: ent
Constant, variable, function or table? /FUNCTION/:  FUNCTION
Name: rp2
Function: bcr*ccr+bmo*cmo+bcu*ccu+bn*cn+bm23*cm23;
POLY_3:
POLY_3: ent func rp02=rp1+rp2;
POLY_3:
POLY_3: eval
Name(s): *
 CC=6.3554801E-2
 CSI=1.3063211
 CMN=1.3039537
 CCR=24.363471
 CNI=20.087675
 CMO=0.28672407
 CCU=0.24116697
 CN=7.0340367E-2
 CFE=52.276793
 CM23=0.48388543
 TC=1079.85
 BC=176.96729
 BSI=59.223483
 BMN=-8.95895
 BCR=-0.455895
 BNI=1.736495
 BMO=2.436495
 BCU=-1.47374
 BN=271.12745
 BM23=62.577975
 AT=1.9577404
 RP1=113.76984
 RP2=38.587774
 RP02=152.35761
POLY_3:
POLY_3: @@ turn off the global minimization calculation and suspend
POLY_3: @@ all phases except fcc#1. This will speed up the calculation
POLY_3: @@ and doesn't affect the results.
POLY_3: advanced
Which option? /STEP_AND_MAP/:  glo
 Settings for global minimization:
   Use global minimization as much as possible /Y/:  n,,,,
POLY_3:
POLY_3: c-s phase
Phase name(s): *
Status: /ENTERED/:  sus
POLY_3:
POLY_3: c-s phase fcc#1=enter 1
POLY_3:
POLY_3: s-c t=500
POLY_3: c-e
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
     7 ITS,  CPU TIME USED   0 SECONDS
POLY_3: l-e,,,
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE6

 Conditions:
 P=1E5, N=1, T=500, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
    W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.44622E+01
 Total Gibbs energy -1.87430E+04,  Enthalpy  9.33796E+03,  Volume  7.00887E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.0809E-03  9.0000E-04 6.3735E-02 -1.1445E+04 SER
 CR                      2.5767E-01  2.4600E-01 2.3975E-01 -5.9371E+03 SER
 CU                      2.0569E-03  2.4000E-03 6.2527E-01 -1.9521E+03 SER
 FE                      5.0808E-01  5.2100E-01 3.3960E-02 -1.4062E+04 SER
 MN                      1.2887E-02  1.3000E-02 6.1504E-06 -4.9883E+04 SER
```

```
 MO                     1.7030E-03  3.0000E-03 6.4768E-02 -1.1378E+04 SER
 N                      2.7217E-03  7.0000E-04 5.4203E-14 -1.2699E+05 SER
 NI                     1.8559E-01  2.0000E-01 9.0077E-04 -2.9152E+04 SER
 SI                     2.5209E-02  1.3000E-02 1.2109E-15 -1.4279E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4462E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  5.21000E-01  SI  1.30000E-02  CU  2.40000E-03
 CR  2.46000E-01  MN  1.30000E-02  C   9.00000E-04
 NI  2.00000E-01  MO  3.00000E-03  N   7.00000E-04
POLY_3: l-st
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT              STATUS    REF. STATE     T(K)           P(Pa)
 VA                     ENTERED   SER
 C                      ENTERED   SER
 CR                     ENTERED   SER
 CU                     ENTERED   SER
 FE                     ENTERED   SER
 MN                     ENTERED   SER
 MO                     ENTERED   SER
 N                      ENTERED   SER
 NI                     ENTERED   SER
 SI                     ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 FCC_A1#1               ENTERED    0.00000000E+00  1.00000000E+00
 SUSPENDED PHASES:
 Z_PHASE SIGMA SIC R_PHASE P_PHASE PI NI3TI NBNI3 MU_PHASE MSI MC_SHP MC_ETA
 M7C3 M6C M5SI3 M5C2 M3SI M3C2 M23C6 LAVES_PHASE_C14 KSI_CARBIDE KAPPA
 HCP_A3#2 HCP_A3#1 GRAPHITE FECN_CHI FE8SI2C FE4N_LP1 FE2SI FCC_A1#2
 DIAMOND_FCC_A4 CR3SI CHI_A12 CEMENTITE BCC_A2 AL4C3 LIQUID GAS
 *** STATUS FOR ALL SPECIES
 C      ENTERED    MN     ENTERED    N3     ENTERED    SIN4/3 ENTERED
 CR     ENTERED    MO     ENTERED    NI     ENTERED    VA     ENTERED
 CU     ENTERED    N      ENTERED    SI     ENTERED
 FE     ENTERED    N2     ENTERED    SI3N4  ENTERED
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-a-v 1 t
Min value /0/:  200
Max value /1/:  1000
Increment /20/:  10
POLY_3:
POLY_3: save tcex44 y
POLY_3: @@ Step in temperature in order to evaluate proof strength
POLY_3: @@ as function of temperature.
POLY_3: step
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    500.000
 POLY has calculated initial equilibrium

 Phase Region from    500.000     for:
     FCC_A1#1
 Terminating at    1000.00
 Calculated    53 equilibria

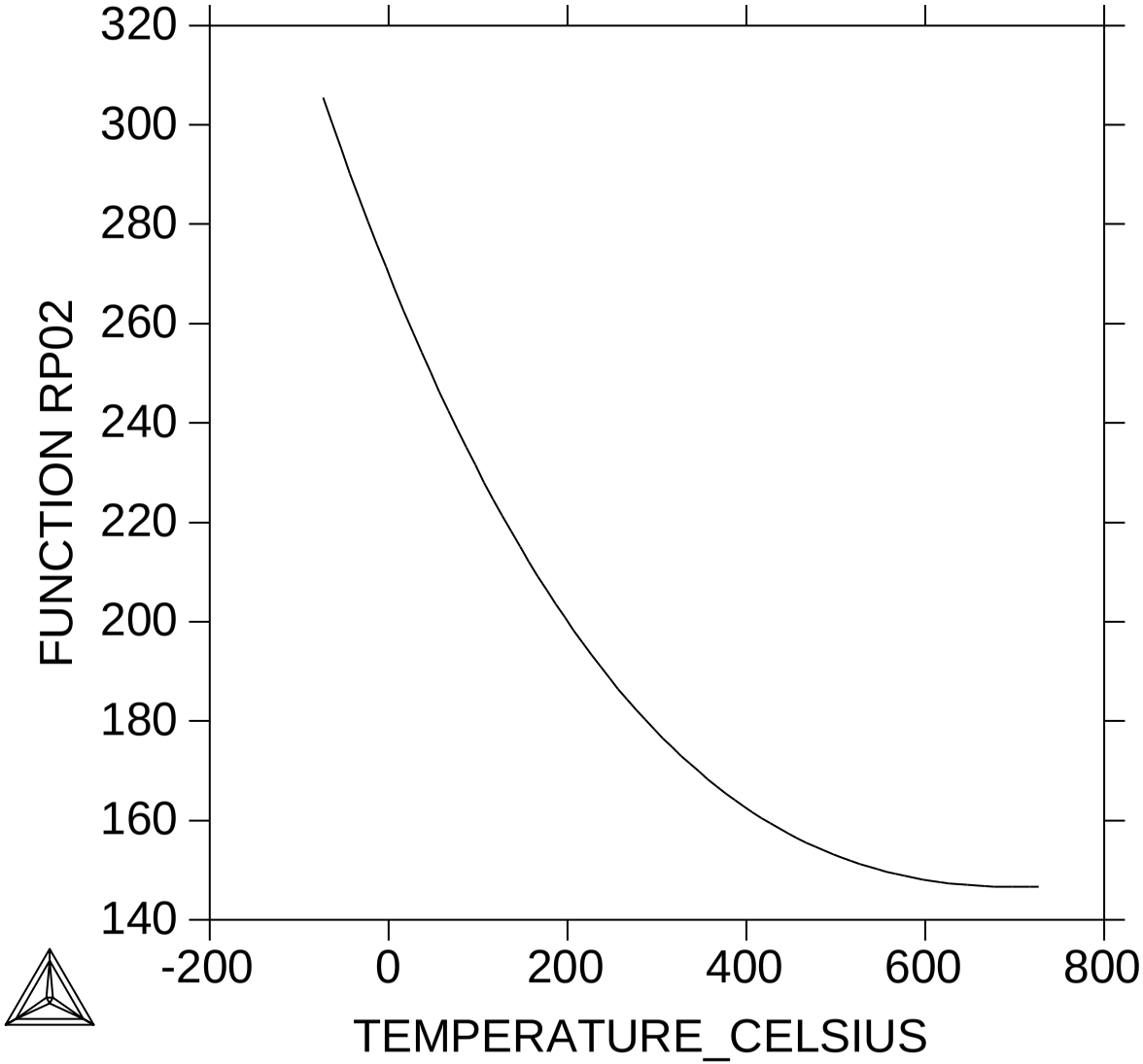
 Phase Region from    500.000     for:
     FCC_A1#1
 Terminating at    200.000
 Calculated    33 equilibria
 *** Buffer saved on file: tcex44.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

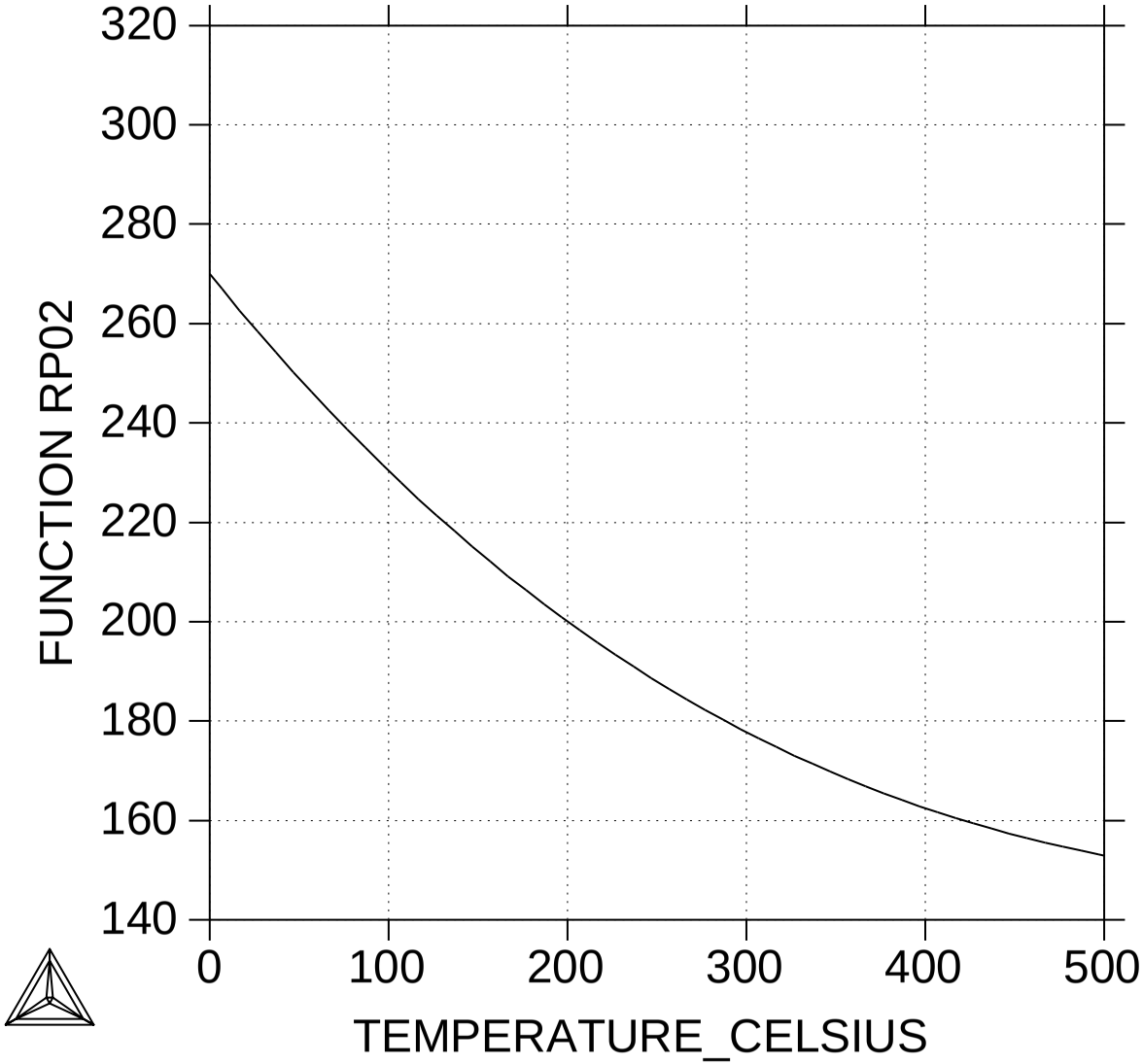
POST: s-d-a y rp02
POST: s-d-a x t-c
POST:
POST: @@ The plot device is set interactively
POST: @#1Plotformat
POST:
POST: s-p-f ##1,,,,,
```

```
POST:
POST: set-title example 44a
POST: plot
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: s-s-s x n 0 500
POST:
POST: set-ras y
POST:
POST: set-title example 44b
POST: plot
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: set-axis-length
AXIS (X, Y OR Z) : x
AXIS LENGTH /11.5/:  20
POST:
POST: set-axis-text-status
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT  (Y OR N) /N/:  n
AXIS TEXT : Proof Strength  (MPa)
POST:
POST: set-axis-text-status
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT  (Y OR N) /N/:  n
AXIS TEXT : Temperature (Celcius)
POST:
POST: set-title example 44c
POST: plot
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: set-plot-option
PLOT HEADER /Y/:  Y
PLOT LOGO /Y/:  Y
PLOT FOOTER /Y/:  Y
WHITE-CONTOURED-PS-CHARS /N/:  N
PLOT REMOTE EXPONENT(S) /Y/:  Y
PLOT SYMBOLS AT NODE POINTS /0/:  0
SYMBOL SIZE /.1/:  .1
WRITE CONDITIONS? /Y/:  n
WRITE DATABASE NAME? /Y/:
Always initiate POST on re-entering: /Y/:  set-title example 44d
POST: plot
POST:
POST: @?<Hit_return_to_continue>
 CPU time           5  seconds
```

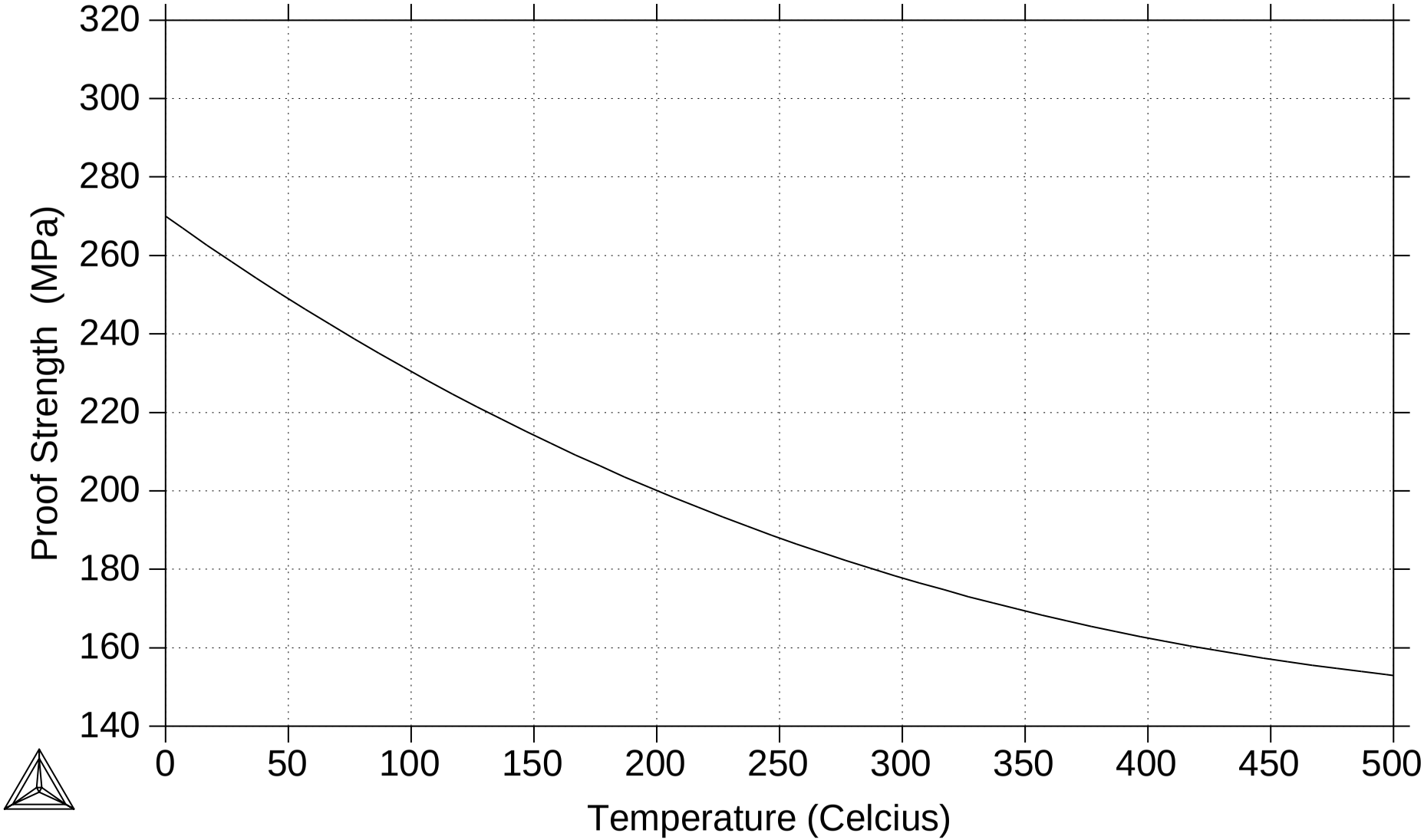
THERMO-CALC (2009.04.27:14.37) :example 44a
DATABASE:TCFE6
P=1E5, N=1, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2, W(MN)=1.3E-2,
W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3;



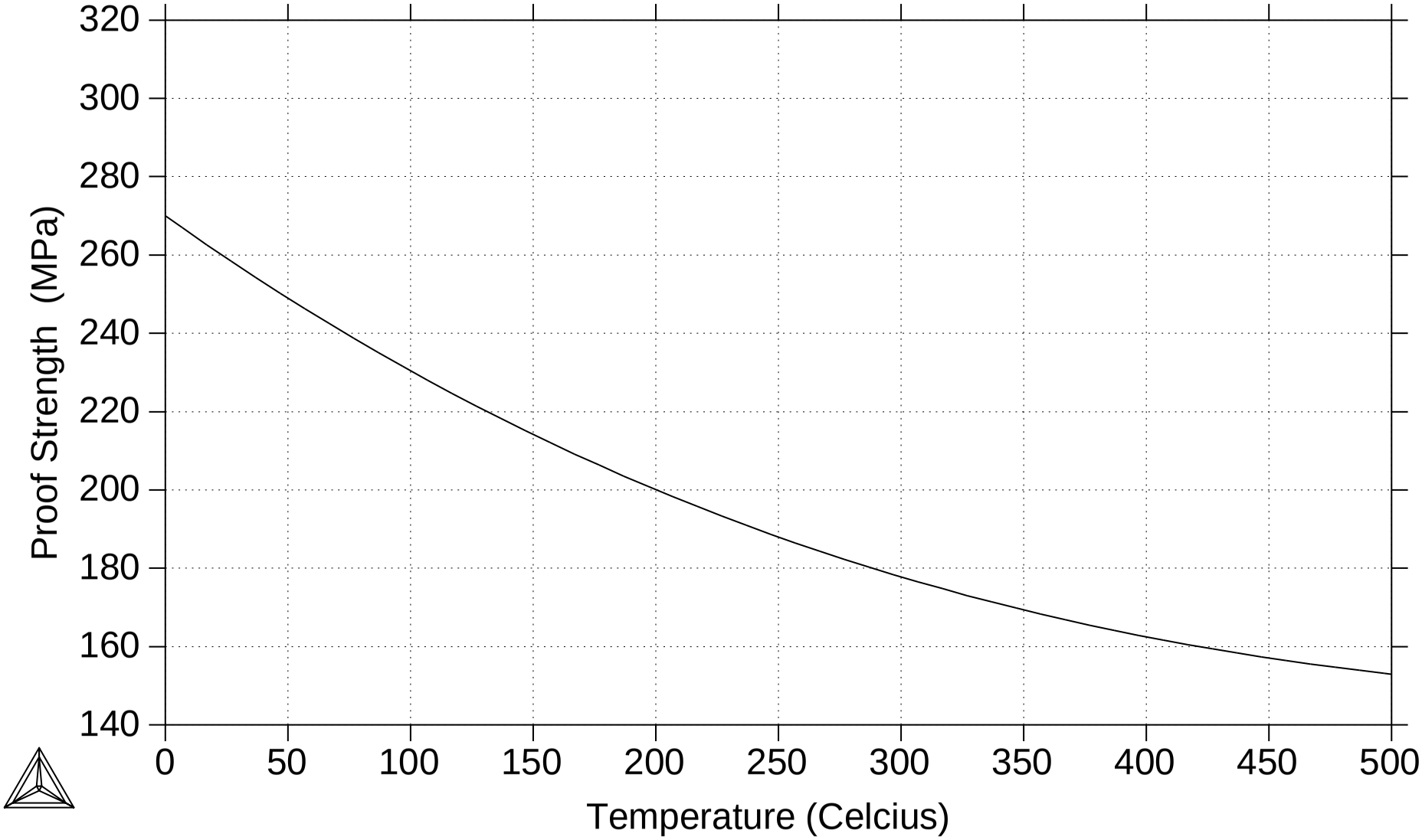
THERMO-CALC (2009.04.27:14.37) :example 44b
DATABASE:TCFE6
P=1E5, N=1, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2, W(MN)=1.3E-2,
W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3;



THERMO-CALC (2009.04.27:14.37) :example 44c
DATABASE:TCFE6
P=1E5, N=1, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2, W(MN)=1.3E-2,
W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3;



THERMO-CALC (2009.04.27:14.37) :example 44c
DATABASE:TCFE6



45

3D-Diagram
with the gamma volume in the Fe-Cr-C system

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ This file calculates the gamma volume in the fe-cr-c system.
SYS: @@ Please note that in order to view the generated file, tcex45.wrl,
SYS: @@ it's necessary to install a WRML(Wirtual Reality Modelling
SYS: @@ Language) viewer to the web browser in use. WRML viwers can be
SYS: @@ downloaded from e.g. www.parallelgraphics.com and www.sim.no
SYS:
SYS: set-log  ex45,,,
SYS:
SYS: @@ Start with calculating the Fe-C side of the diagram
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw ptern
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN: def-sys fe c
   ... the command in full is DEFINE_SYSTEM
 FE                      C  DEFINED
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
       C-FE'
  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
      Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'W. Huang, TRITA-MAC 441 (1990), Fe-Mn-V-C '
 -OK-
TDB_PTERN:
TDB_PTERN: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
```

```
 Calculated          553  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 800 1800 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3:
POLY_3: save tcex45 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
 Generating start point  31
 Generating start point  32

 Phase region boundary   1 at:   5.236E-01  1.137E+03
    FCC_A1
  ** GRAPHITE
```

```
 *** Buffer saved on file: tcex45.POLY3
 Calculated.           14  equilibria

 Phase region boundary   2 at:   5.155E-01  1.011E+03
  ** BCC_A2
     FCC_A1
  ** GRAPHITE

 Phase region boundary   3 at:   1.587E-02  1.011E+03
  ** BCC_A2
     FCC_A1
 Calculated           33  equilibria

 Phase region boundary   4 at:   5.155E-01  1.011E+03
     FCC_A1
  ** GRAPHITE
 Calculated.           43  equilibria

       :
       :
       :

 Phase region boundary  10 at:   5.236E-01  1.137E+03
     FCC_A1
  ** GRAPHITE
 Calculated.           14  equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   5.236E-01  1.137E+03
     FCC_A1
  ** GRAPHITE
 Calculated.           30  equilibria
 Terminating at known equilibrium

 Phase region boundary  12 at:   1.216E-01  1.463E+03
  ** LIQUID
     FCC_A1
 Calculated.            5  equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   1.216E-01  1.463E+03
  ** LIQUID
     FCC_A1
 Calculated.           32  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex45.POLY3
 CPU time for mapping           2  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x w(fcc,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the fcc phase, in the second Cr content which is "zero"
POST: @@ here, and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(fcc,c),zero,T
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fec.tab
   ... the command in full is TABULATE
```

```
POST: back
POLY_3:
POLY_3: @@ Next step is to calculate the Fe-Cr side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_PTERN: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
TDB_PTERN: de-sys fe cr
   ... the command in full is DEFINE_SYSTEM
 FE                    CR  DEFINED
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
      (1986); CR-FE'
 -OK-
TDB_PTERN:
TDB_PTERN: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          549  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 800 1800 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3:
POLY_3: save tcex45 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
```

```
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Working hard
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   1.067E-02  1.169E+03
     BCC_A2
  ** FCC_A1
 Calculated           11  equilibria

 Phase region boundary   2 at:   1.067E-02  1.169E+03
     BCC_A2
  ** FCC_A1
 Calculated           92  equilibria

 Phase region boundary   3 at:   4.322E-02  1.137E+03
     BCC_A2
  ** FCC_A1
 Calculated           89  equilibria

 Phase region boundary   4 at:   4.322E-02  1.137E+03
     BCC_A2
  ** FCC_A1
 Calculated           18  equilibria

       :
       :
       :

 Phase region boundary   9 at:   1.051E-01  1.463E+03
     BCC_A2
  ** FCC_A1
 Calculated           58  equilibria

 Phase region boundary  10 at:   1.051E-01  1.463E+03
     BCC_A2
```

```
 ** FCC_A1
 Calculated           43  equilibria

 Phase region boundary  11 at:   9.912E-03  1.665E+03
    BCC_A2
 ** FCC_A1
 Calculated           14  equilibria

 Phase region boundary  12 at:   9.912E-03  1.665E+03
    BCC_A2
 ** FCC_A1
 Calculated           86  equilibria
 *** BUFFER SAVED ON FILE: tcex45.POLY3
 CPU time for mapping           2  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x W(fcc,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the fcc phase, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): zero,W(fcc,cr),T
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fecr.tab
   ... the command in full is TABULATE
POST:
POST: @@ Now let's calculate the ternary projection of the fcc phase
POST: back
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_PTERN: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
TDB_PTERN: de-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                    CR                    C
   DEFINED
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
  'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
```

```
      C-FE'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
      (1986); CR-FE'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
      Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'
  'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'W. Huang, TRITA-MAC 441 (1990), Fe-Mn-V-C '
 -OK-
TDB_PTERN:
TDB_PTERN: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: se-con t=1050
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1100
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1200
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            1  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1300
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
```

```
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1400
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1500
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1600
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1700
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3:
POLY_3: save fecrc y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
```

```
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17

 Phase region boundary   1 at:   9.164E-03  1.915E-02
  ** BCC_A2
     FCC_A1#1
 Calculated           13  equilibria

 Phase region boundary   2 at:   1.589E-01  2.205E-01
     FCC_A1#1
  ** M7C3
 Calculated.            6  equilibria

 Phase region boundary   3 at:   1.646E-01  1.736E-01
  ** CEMENTITE
     FCC_A1#1
  ** M7C3

 Phase region boundary   4 at:   1.396E-01  8.004E-02
  ** CEMENTITE
     FCC_A1#1
 Calculated.            7  equilibria

       :
       :
       :

 Phase region boundary  67 at:   4.442E-02  2.213E-02
  ** LIQUID
     FCC_A1#1
 Calculated.           13  equilibria

 Phase region boundary  68 at:   3.037E-02  1.325E-01
  ** LIQUID
  ** BCC_A2
     FCC_A1#1

 Phase region boundary  69 at:   1.198E-02  1.224E-01
  ** BCC_A2
     FCC_A1#1
 Calculated           26  equilibria

 Phase region boundary  70 at:   3.037E-02  1.325E-01
  ** LIQUID
     FCC_A1#1
 Calculated           28  equilibria
 *** BUFFER SAVED ON FILE: fecrc.POLY3
 CPU time for mapping           7  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x W(fcc,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(fcc,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: back
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
```

```
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 3 T 800 2000 5
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: se-con x(cr)=.1
   ... the command in full is SET_CONDITION
POLY_3: se-con x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-con t=1373
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: ad-ini 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3:
POLY_3: map
 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18

 Phase region boundary   1 at:   1.777E-02  2.292E-02  1.050E+03
  ** BCC_A2
     FCC_A1#1
  ** M7C3
 CALCULATED     9 EQUILIBRIA

 Phase region boundary   2 at:   2.658E-02  1.344E-02  1.022E+03
  ** BCC_A2
     CEMENTITE
     FCC_A1#1
  ** M7C3
 SKIPPING LINE WITHOUT FCC_A1#1

 Phase region boundary   2 at:   2.658E-02  1.344E-02  1.022E+03
  ** BCC_A2
  ** CEMENTITE
     FCC_A1#1
 CALCULATED     6 EQUILIBRIA

 Phase region boundary   2 at:   3.184E-02  4.319E-03  1.007E+03
  ** BCC_A2
```

```
 ** CEMENTITE
    FCC_A1#1
    GRAPHITE
SKIPPING LINE WITHOUT FCC_A1#1

      :
      :
      :

Phase region boundary   2 at:   2.521E-02  2.000E-02  1.436E+03
 ** LIQUID
 ** CEMENTITE
    FCC_A1#1
Terminating at diagram limit
CALCULATED     7 EQUILIBRIA

Phase region boundary   2 at:   2.521E-02  2.000E-02  1.436E+03
 ** LIQUID
 ** CEMENTITE
    FCC_A1#1
Terminating at known equilibrium
CALCULATED     6 EQUILIBRIA

Phase region boundary   2 at:   3.131E-02  1.000E-01  1.176E+03
    FCC_A1#1
 ** M23C6
 ** M7C3
*** Buffer saved on file: fecrc.POLY3
Terminating at known equilibrium
CALCULATED    21 EQUILIBRIA

Phase region boundary   2 at:   3.131E-02  1.000E-01  1.176E+03
    FCC_A1#1
 ** M23C6
 ** M7C3
Terminating at known equilibrium
*** LAST BUFFER SAVED ON FILE: fecrc.POLY3
CPU time for mapping           3  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

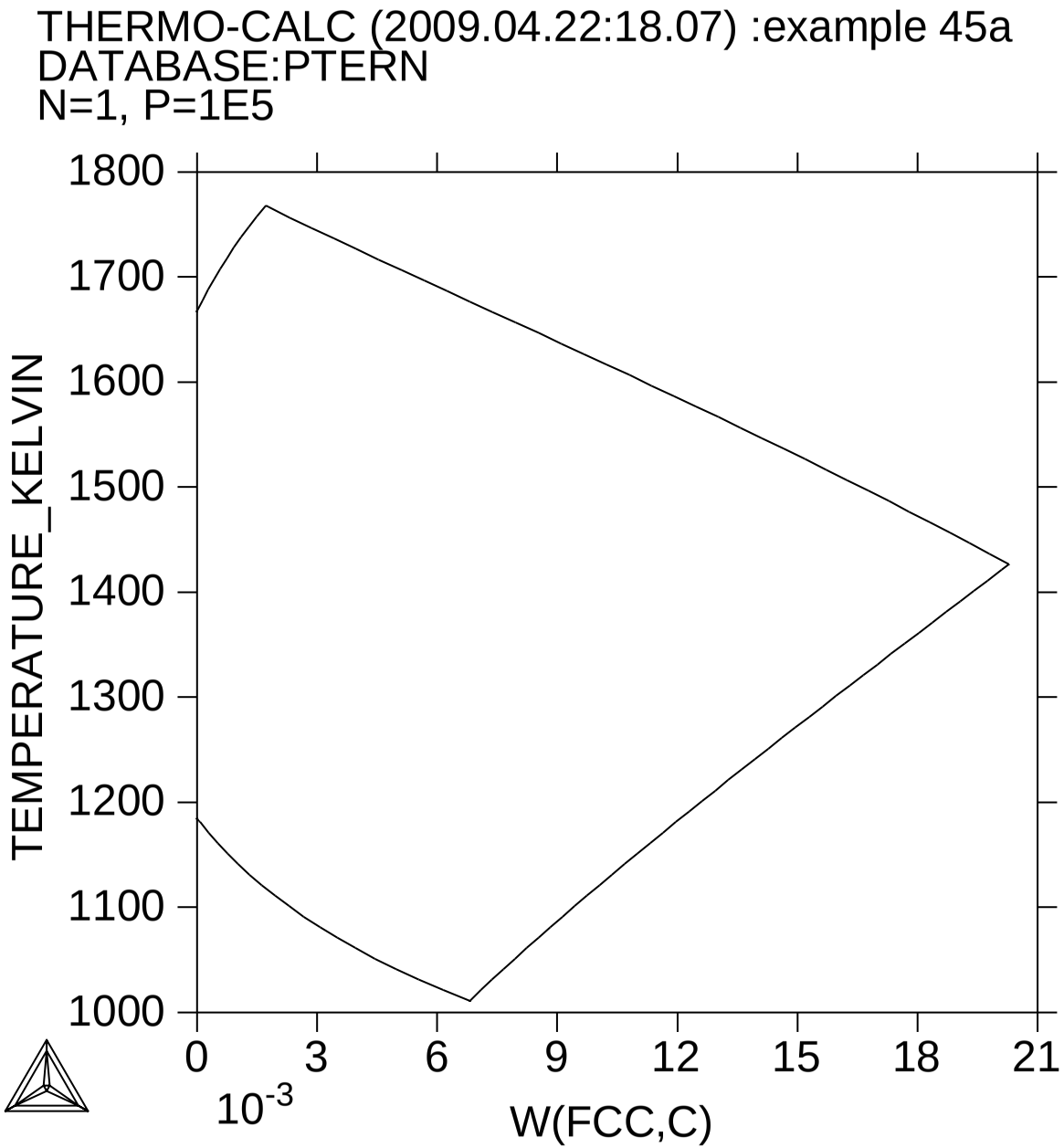
 Setting automatic diagram axis

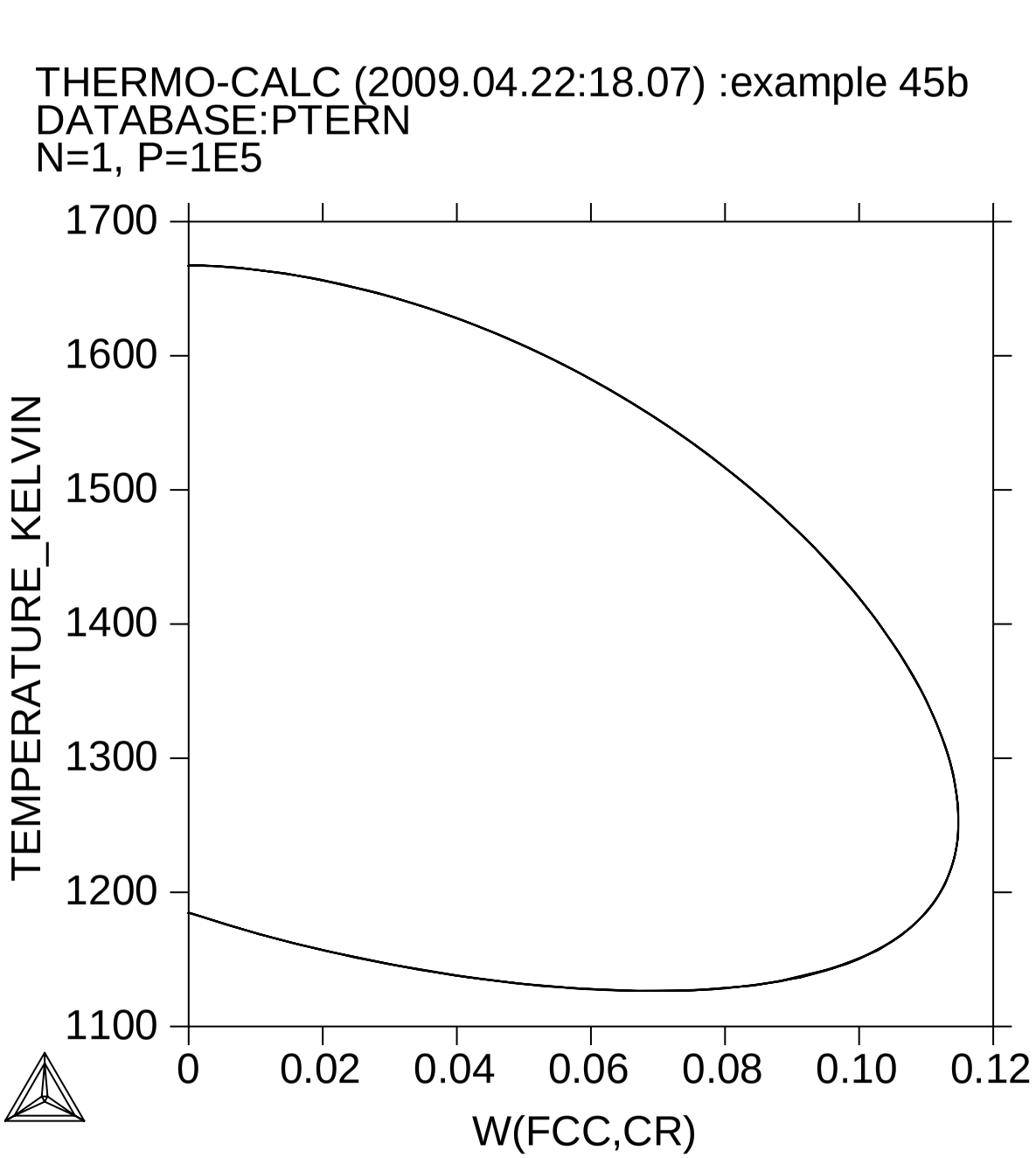
POST: s-d-a x W(fcc,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(fcc,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Enter the table for the calculated data.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(fcc,c),W(fcc,cr),T;
POST:
POST: tab tab1 fecrc.tab
   ... the command in full is TABULATE
POST:
POST: @@ Set the axis variables and the axis text for the final diagram
POST: s-a-t-s x n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac C
POST: s-a-t-s y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac Cr
POST:
POST: s-d-a z temp-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-t-s z n
```

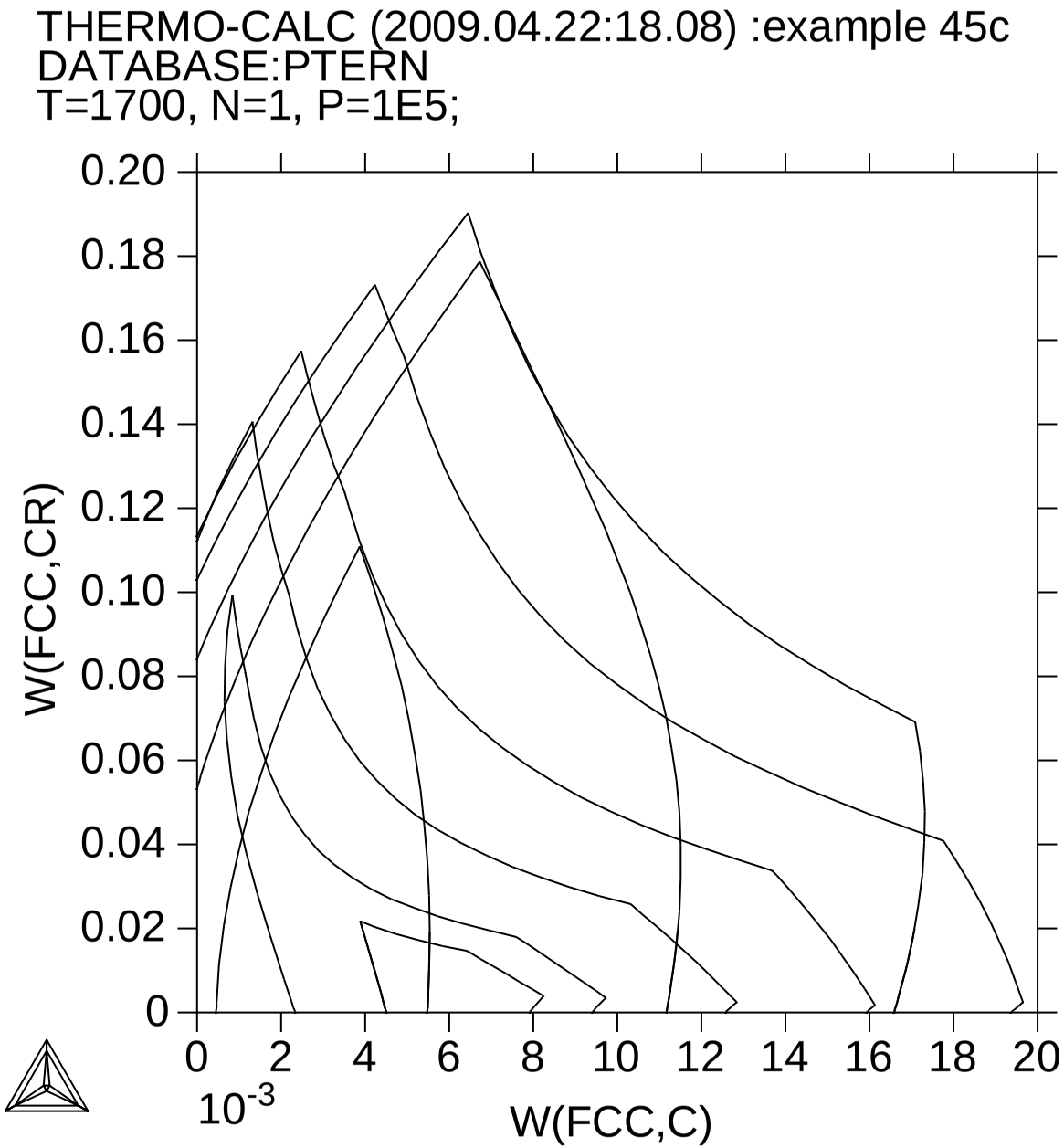
```
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Temp C
POST:
POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data
POST: @@ from the different tables created and saved. This is accomplished
POST: @@ using the command "CREATE_3D_DIAGRAM". Also define the scaling
POST: @@ to be used in the 3D-diagram.
POST: cre-3d
   ... the command in full is CREATE_3D_PLOTFILE
Use current WORKSPACE (WS), TAB files or BOTH: /WS/:  BOTH
 The table must contain values for X,Y and Z axis
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    TEMP_C=T-273.15
 DEFINED TABLES
    TAB1=W(FCC_A1#1,C), W(FCC_A1#1,CR), T
Table Name: tab1
Give TAB filename: /Cancel_to_finish/:  fec.tab fecr.tab Cancel_to_finish
Output file: /3Dplot/:  tcex45.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/:  .02
Y-AXIS SCALING FROM 0.0 TO YMAX /1/:  .20
Z-AXIS SCALING, GIVE ZMIN /0/:  1000
Z-AXIS SCALING, GIVE ZMAX /2000/:  2000
 It is possible to combine files by:
 Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

 Processing fec.tab
  2.2511500E-11 <X<  2.0285400E-02
   0.000000     <Y<   0.000000
   1011.170     <Z<   1767.760

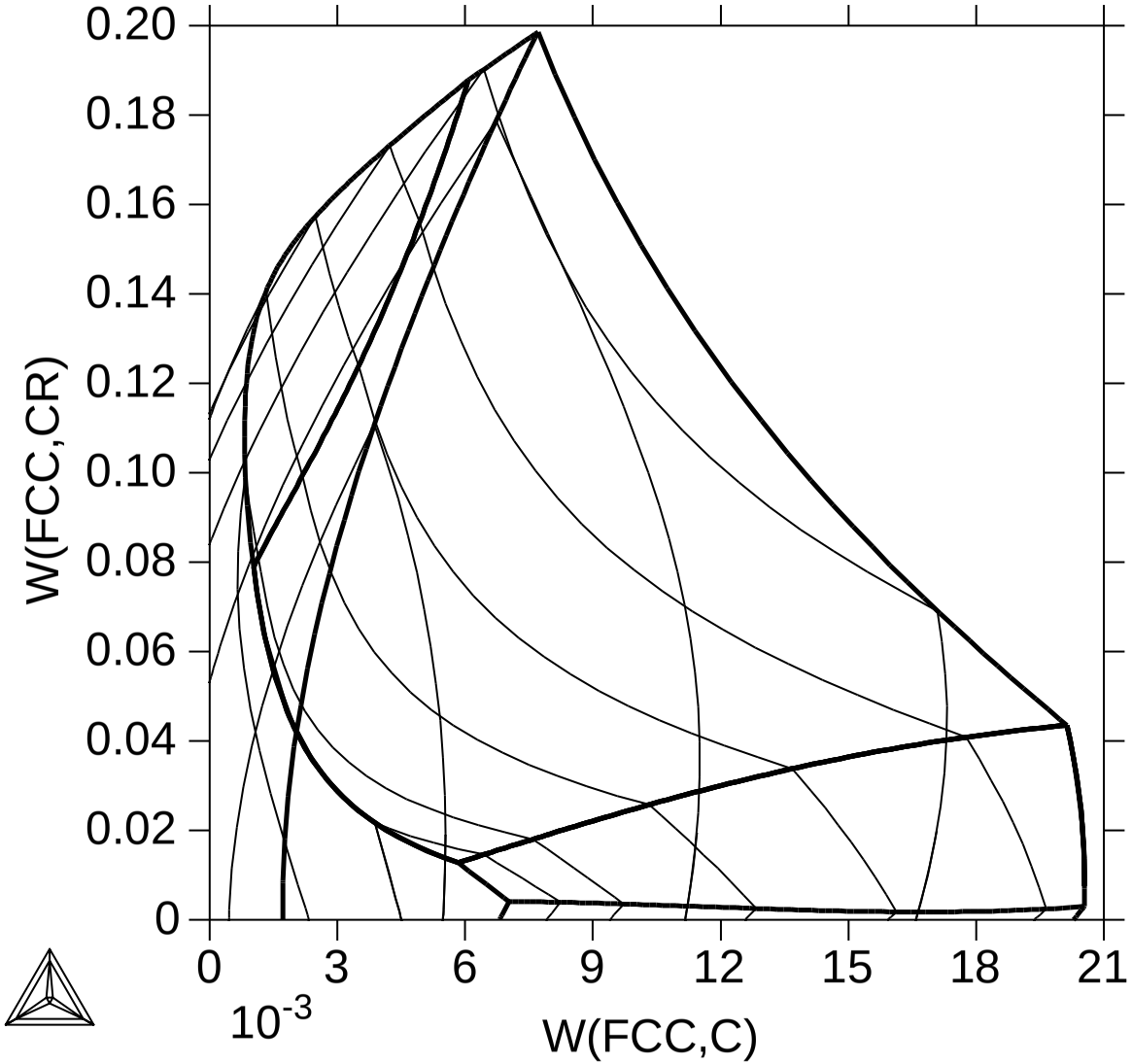
 Processing fecr.tab
   0.000000     <X<   0.000000
  1.3388500E-09 <Y<  0.1148190
   1126.310     <Z<   1667.480
POST:
POST:
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           16  seconds
```


THERMO-CALC (2009.04.22:18.07) :example 45a
DATABASE:PTERN
N=1, P=1E5
TEMPERATURE_KELVIN
1800
1700
1600
1500
1400
1300
1200
1100
1000
0
3
6
9
12
15
18
21
10-3
W(FCC,C)


THERMO-CALC (2009.04.22:18.07) :example 45b
DATABASE:PTERN
N=1, P=1E5
TEMPERATURE_KELVIN
1700
1600
1500
1400
1300
1200
1100
0
0.02
0.04
0.06
0.08
0.10
0.12
W(FCC,CR)

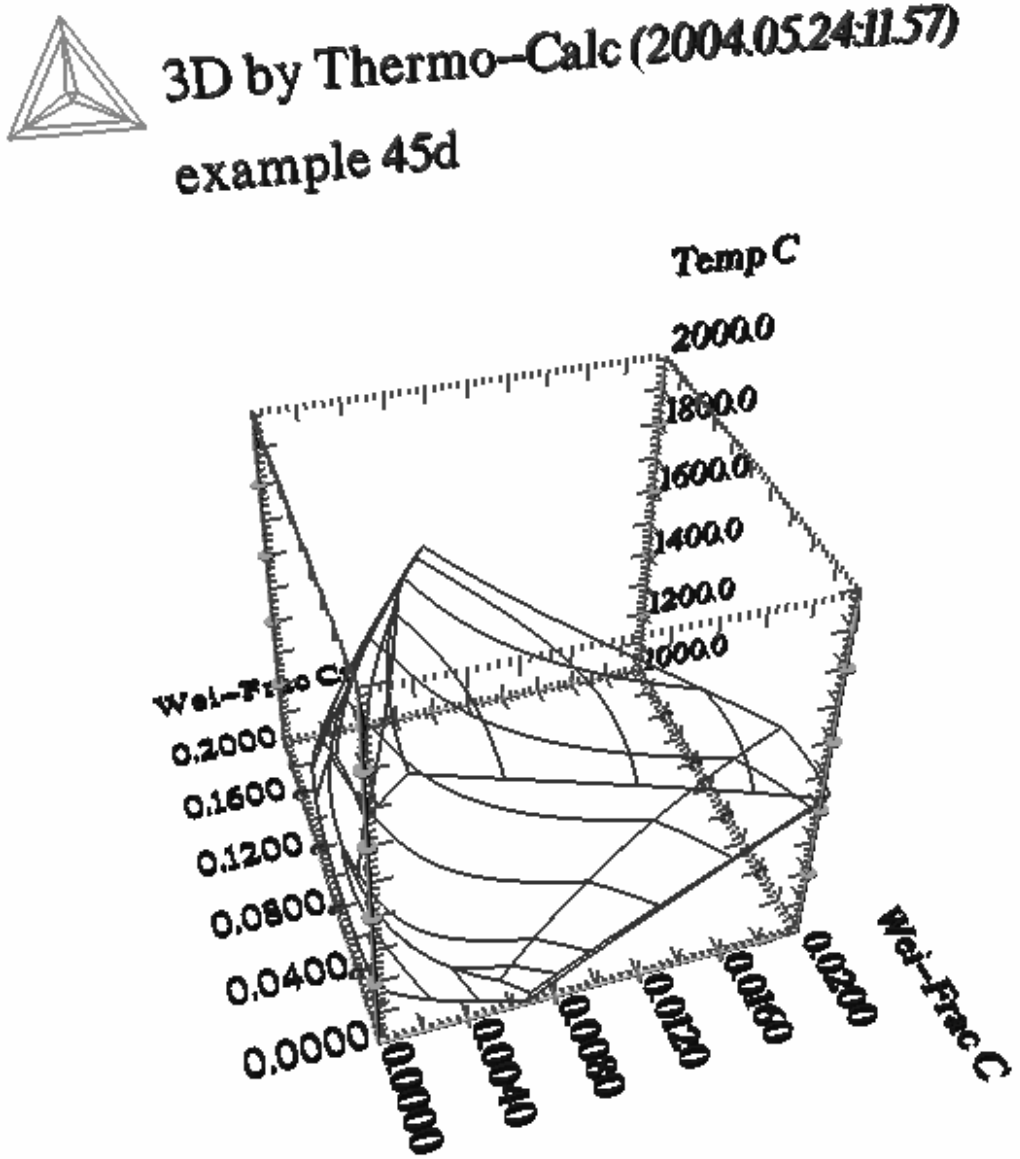

THERMO-CALC (2009.04.22:18.08) :example 45c
DATABASE:PTERN
T=1700, N=1, P=1E5;
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0
W(FCC,CR)
0
2
4
6
8
10
12
14
16
18
20
10-3
W(FCC,C)

THERMO-CALC (2009.04.22:18.08) :example 45d
DATABASE:PTERN
N=1., P=1E5;



VRMLView [TCEX45.WRL]

File View SpecialFX Settings Camera Lights Windows Help



Ready!

start | Eudora - [Britt-Mari... | tcex45 | Temp | Microsoft PowerPoi... | VRMLView [TCEX45... | SV | 12:47

46

3D-Diagram
with the liquidus surface of the Fe-Cr-C system

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@This file calculates the Liquidus surface in the FE-CR-C system
SYS: @@ Please note that in order to view the generated files, tcex46_tri.wrl
SYS: @@ and tcex46_sqrt, it's necessary to install a WRML(Wirtual Reality
SYS: @@ Modelling Language) viewer to the web browser in use. WRML viwers
SYS: @@ can be downloaded from e.g. www.parallelgraphics.com and
SYS: @@ www.sim.no
SYS:
SYS: set-log ex46,,
SYS:
SYS: @@ Start by calculating the Fe-C side of the diagram
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw tcfe6
   ... the command in full is SWITCH_DATABASE
TDB_TCFE6: de-sys fe c
   ... the command in full is DEFINE_SYSTEM
 FE                      C  DEFINED
TDB_TCFE6: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    KSI_CARBIDE             A1_KAPPA
 KAPPA                   FE4N_LP1                FECN_CHI
 LAVES_PHASE_C14  REJECTED
TDB_TCFE6: res-ph fcc,bcc,cem,gra,liq
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  CEMENTITE
 GRAPHITE                LIQUID:L  RESTORED
TDB_TCFE6: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 -OK-
TDB_TCFE6:
TDB_TCFE6: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1973
```

```
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          413  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1300 5000 20
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3:
POLY_3: save tcex46 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   1.982E-02  1.759E+03
  ** LIQUID
```

```
    FCC_A1
 *** Buffer saved on file: tcex46.POLY3
 Calculated.            2  equilibria

 Phase region boundary   2 at:   1.599E-02  1.768E+03
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary   3 at:   1.417E-02  1.768E+03
     LIQUID
  ** BCC_A2
 Calculated           15  equilibria

 Phase region boundary   4 at:   1.599E-02  1.768E+03
  ** LIQUID
     FCC_A1
 Calculated.           19  equilibria

       :
       :
       :

 Phase region boundary  20 at:   8.317E-01  4.174E+03
     LIQUID
  ** GRAPHITE
 Calculated.          147  equilibria
 Terminating at known equilibrium

 Phase region boundary  21 at:   8.317E-01  4.174E+03
     LIQUID
  ** GRAPHITE
 Calculated           43  equilibria

 Phase region boundary  22 at:   9.950E-01  4.749E+03
     LIQUID
  ** GRAPHITE
 Calculated.          179  equilibria
 Terminating at known equilibrium

 Phase region boundary  23 at:   9.950E-01  4.749E+03
     LIQUID
  ** GRAPHITE
 Calculated           18  equilibria
 *** BUFFER SAVED ON FILE: tcex46.POLY3
 CPU time for mapping           1  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x w(liq,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46a
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(liq,c),zero,Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fec_liq.tab
   ... the command in full is TABULATE
POST: back
```

```
POLY_3:
POLY_3: @@ Next calculate the Fe-Cr side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE6: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 IONIC_LIQ:Y            L12_FCC                B2_BCC
 B2_VACANCY             HIGH_SIGMA             DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
TDB_TCFE6: de-sys fe cr
   ... the command in full is DEFINE_SYSTEM
 FE                     CR  DEFINED
TDB_TCFE6: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L               BCC_A2                 FCC_A1
 HCP_A3                 A1_KAPPA               KAPPA
 SIGMA                  CHI_A12                LAVES_PHASE_C14
 CR3SI  REJECTED
TDB_TCFE6: res-ph bcc,liq
   ... the command in full is RESTORE
 BCC_A2                 LIQUID:L  RESTORED
TDB_TCFE6: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
 -OK-
TDB_TCFE6:
TDB_TCFE6: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=2373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          274  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1500 2400 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3:
POLY_3: save tcex46 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
```

```
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24

 Phase region boundary   1 at:   1.039E-02  1.809E+03
  ** LIQUID
     BCC_A2
 Calculated           14  equilibria

 Phase region boundary   2 at:   1.039E-02  1.809E+03
  ** LIQUID
     BCC_A2
 Calculated          110  equilibria

 Phase region boundary   3 at:   3.280E-01  1.802E+03
  ** LIQUID
     BCC_A2
 Calculated           43  equilibria

 Phase region boundary   4 at:   3.280E-01  1.802E+03
  ** LIQUID
     BCC_A2
 Calculated           81  equilibria

       :
       :
       :
```

```
 Phase region boundary  21 at:   6.881E-01  2.007E+03
    LIQUID
  ** BCC_A2
 Calculated           83  equilibria

 Phase region boundary  22 at:   6.881E-01  2.007E+03
    LIQUID
  ** BCC_A2
 Calculated           41  equilibria

 Phase region boundary  23 at:   9.910E-01  2.176E+03
    LIQUID
  ** BCC_A2
 Calculated          106  equilibria

 Phase region boundary  24 at:   9.910E-01  2.176E+03
    LIQUID
  ** BCC_A2
 Calculated           14  equilibria
 *** BUFFER SAVED ON FILE: tcex46.POLY3
 CPU time for mapping           2  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x W(liq,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): zero,W(liq,cr),Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fecr_liq.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Then calculate the Cr-C side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE6: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
TDB_TCFE6: de-sys c cr
   ... the command in full is DEFINE_SYSTEM
 C                       CR  DEFINED
TDB_TCFE6: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M3C2                    KSI_CARBIDE             FE4N_LP1
 SIGMA                   CHI_A12                 LAVES_PHASE_C14
 CR3SI  REJECTED
TDB_TCFE6: res-ph bcc,liq,grap,m23,m7c,m3c2
   ... the command in full is RESTORE
 BCC_A2                  LIQUID:L                GRAPHITE
```

```
 M23C6                  M7C3                   M3C2
   RESTORED
TDB_TCFE6: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'P. Villars and L.D. Calvert (1985). Pearson´s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
 -OK-
TDB_TCFE6:
TDB_TCFE6: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=2373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=1.5e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          278  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1500 5000 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3:
POLY_3: save tcex46 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3:
POLY_3: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
```

```
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28

 Phase region boundary   1 at:   2.762E-01  2.670E+03
     LIQUID
  ** GRAPHITE
 Calculated.           61  equilibria

 Phase region boundary   2 at:   3.108E-01  2.077E+03
     LIQUID
  ** GRAPHITE
  ** M3C2

 Phase region boundary   3 at:   6.108E-01  2.077E+03
     LIQUID
  ** M3C2
 Calculated.            7  equilibria

 Phase region boundary   4 at:   6.354E-01  2.018E+03
     LIQUID
  ** M3C2
  ** M7C3

       :
       :
       :

 Phase region boundary  22 at:   6.317E-01  2.031E+03
     LIQUID
  ** M3C2
 Calculated.            7  equilibria
 Terminating at known equilibrium

 Phase region boundary  23 at:   6.317E-01  2.031E+03
     LIQUID
  ** M3C2
 Calculated.            3  equilibria
 Terminating at known equilibrium

 Phase region boundary  24 at:   9.949E-01  2.162E+03
```

```
    LIQUID
  ** BCC_A2
 Calculated.           38  equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   9.949E-01  2.162E+03
    LIQUID
  ** BCC_A2
 Calculated           14  equilibria
 *** BUFFER SAVED ON FILE: tcex46.POLY3
 CPU time for mapping           2  seconds
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x w(liq,C)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y temp-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(liq,c),W(liq,cr),Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tab1 crc_liq.tab
   ... the command in full is TABULATE
POST:
POST: back
POLY_3: @@ Finnaly, calculate a ternary projection of the Fe-Cr-C system
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE6: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 IONIC_LIQ:Y            L12_FCC                B2_BCC
 B2_VACANCY             HIGH_SIGMA             DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
TDB_TCFE6: de-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                     CR                     C
   DEFINED
TDB_TCFE6: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L               BCC_A2                 FCC_A1
 HCP_A3                 DIAMOND_FCC_A4         GRAPHITE
 CEMENTITE              M23C6                  M7C3
 M5C2                   M3C2                   KSI_CARBIDE
 A1_KAPPA               KAPPA                  FE4N_LP1
 FECN_CHI               SIGMA                  CHI_A12
 LAVES_PHASE_C14        CR3SI  REJECTED
TDB_TCFE6: res-ph liq,fcc,bcc,m23,m7c,m3c2,gra,cem
   ... the command in full is RESTORE
 LIQUID:L               FCC_A1                 BCC_A2
 M23C6                  M7C3                   M3C2
 GRAPHITE               CEMENTITE  RESTORED
TDB_TCFE6: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
```

```
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
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  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'B.-J. Lee, Calphad (1993); revison of Fe-Cr and Fe-Ni liquid'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
      (1986); CR-FE'
  'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
  'P. Villars and L.D. Calvert (1985). Pearson´s handbook of
      crystallographic data for intermetallic phases. Metals park, Ohio.
      American Society for Metals; Molar volumes'
 -OK-
TDB_TCFE6:
TDB_TCFE6: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            1  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: se-con t=1600
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1700
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
```

```
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1800
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2100
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2200
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=9e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: se-con t=1900
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
```

```
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2000
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2100
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3:
POLY_3: save fecrc y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard

 Phase region boundary   1 at:   8.271E-02  2.328E-02
  ** LIQUID
     FCC_A1#1
 Calculated           11  equilibria

 Phase region boundary   2 at:   8.271E-02  2.328E-02
  ** LIQUID
     FCC_A1#1
 Calculated.           23  equilibria
```

```
 Phase region boundary   3 at:   6.085E-02  2.377E-01
  ** LIQUID
  ** BCC_A2
     FCC_A1#1

 Phase region boundary   4 at:   4.944E-02  2.509E-01
     LIQUID
  ** BCC_A2
 Calculated.           22  equilibria

       :
       :
       :

 Phase region boundary  52 at:   5.190E-03  7.168E-01
     LIQUID
  ** BCC_A2
 Calculated           20  equilibria

 Phase region boundary  53 at:   5.190E-03  7.168E-01
     LIQUID
  ** BCC_A2
 Calculated           40  equilibria

 Phase region boundary  54 at:   5.138E-03  8.727E-01
     LIQUID
  ** BCC_A2
 Calculated           26  equilibria

 Phase region boundary  55 at:   5.138E-03  8.727E-01
     LIQUID
  ** BCC_A2
 Calculated           30  equilibria
 *** BUFFER SAVED ON FILE: fecrc.POLY3
 CPU time for mapping           9  seconds
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 3 T 1000 3000 8
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: se-con x(cr)=.6
   ... the command in full is SET_CONDITION
POLY_3: se-con x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-con t=1873
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7710  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: ad-ini 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  liq
POLY_3:
POLY_3: map
 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
```

```
Generating start point   5
Generating start point   6
Generating start point   7
Generating start point   8
Generating start point   9
Generating start point  10
Working hard
Generating start point  11
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16

Phase region boundary   1 at:   5.118E-02  2.000E-02  1.446E+03
 ** LIQUID
 ** CEMENTITE
    FCC_A1#1
Terminating at diagram limit
CALCULATED     7 EQUILIBRIA

Phase region boundary   2 at:   5.118E-02  2.000E-02  1.446E+03
 ** LIQUID
 ** CEMENTITE
    FCC_A1#1
CALCULATED     6 EQUILIBRIA

Phase region boundary   2 at:   8.299E-02  4.133E-02  1.467E+03
 ** LIQUID
 ** CEMENTITE
    FCC_A1#1
    M7C3

Phase region boundary   2 at:   3.000E-01  2.339E-01  1.467E+03
 ** LIQUID
 ** CEMENTITE
    M7C3
Terminating at known equilibrium
CALCULATED     3 EQUILIBRIA

      :
      :
      :

Phase region boundary   2 at:   1.036E-01  4.168E-01  1.582E+03
    LIQUID
 ** BCC_A2
 ** M23C6
    M7C3
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   1.036E-01  4.168E-01  1.582E+03
    LIQUID
 ** BCC_A2
 ** M7C3
Terminating at known equilibrium
CALCULATED    13 EQUILIBRIA

Phase region boundary   2 at:   1.036E-01  4.168E-01  1.582E+03
    LIQUID
 ** M23C6
 ** M7C3
*** SORRY CANNOT CONTINUE ***    4

CALCULATED    47 EQUILIBRIA

Phase region boundary   2 at:   3.427E-02  6.000E-01  1.660E+03
    LIQUID
 ** BCC_A2
 ** M23C6
*** SORRY CANNOT CONTINUE ***    4

*** LAST BUFFER SAVED ON FILE: fecrc.POLY3
CPU time for mapping           5  seconds
```

```
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x W(liq,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(liq,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: @?<Hit_return_to_continue>
POST: @@ Enter the table for the calculated data.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): W(liq,c),W(liq,cr),Temp_c;
POST:
POST: @@ Save the table on file
POST: tab tab1 fecrc_liq.tab
   ... the command in full is TABULATE
POST:
POST: @@ Set the axis variables and the axis text for the final diagram
POST: s-a-t-s x n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac C
POST: s-a-t-s y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac Cr
POST:
POST: s-d-a z temp-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-t-s z n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Temp C
POST:
POST: @@ Specify the diagram type to be traingular
POST: s-d-t y,,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST:
POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data
POST: @@ from the different tables created and saved. This is accomplished
POST: @@ using the command "CREATE_3D_DIAGRAM". Also define the scaling
POST: @@ to be used in the 3D-diagram.
POST: cre-3d
   ... the command in full is CREATE_3D_PLOTFILE
Use current WORKSPACE (WS), TAB files or BOTH: /WS/:  BOTH
 The table must contain values for X,Y and Z axis
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    TEMP_C=T-273.15
 DEFINED TABLES
    TAB1=W(LIQUID,C), W(LIQUID,CR), TEMP_C
Table Name: tab1
Give TAB filename: /Cancel_to_finish/:  fec_liq.tab fecr_liq.tab crc_liq.tab Cancel_to
Output file: /3Dplot/:  tcex46_tri.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/:  1
Y-AXIS SCALING FROM 0.0 TO YMAX /1/:  1
Z-AXIS SCALING, GIVE ZMIN /0/:  1200
Z-AXIS SCALING, GIVE ZMAX /2000/:  4600
 It is possible to combine files by:
 Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

 Processing fec_liq.tab
  3.4429100E-09 <X<   1.000000
   0.000000     <Y<   0.000000
   1153.440     <Z<   4500.070

 Processing fecr_liq.tab
```

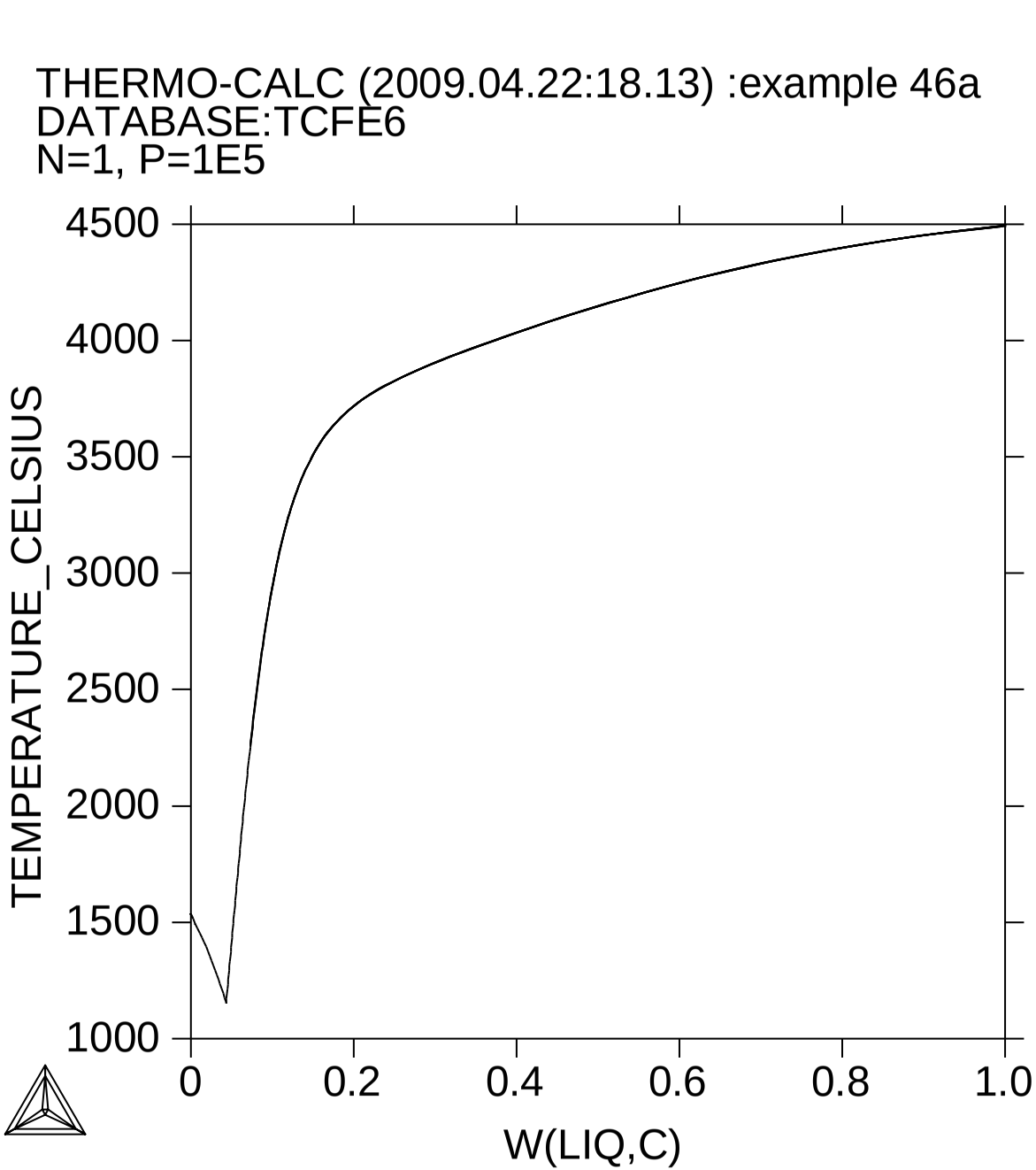
```
   0.000000     <X<   0.000000
  1.1746299E-09 <Y<   1.000000
   1515.560     <Z<   1919.760

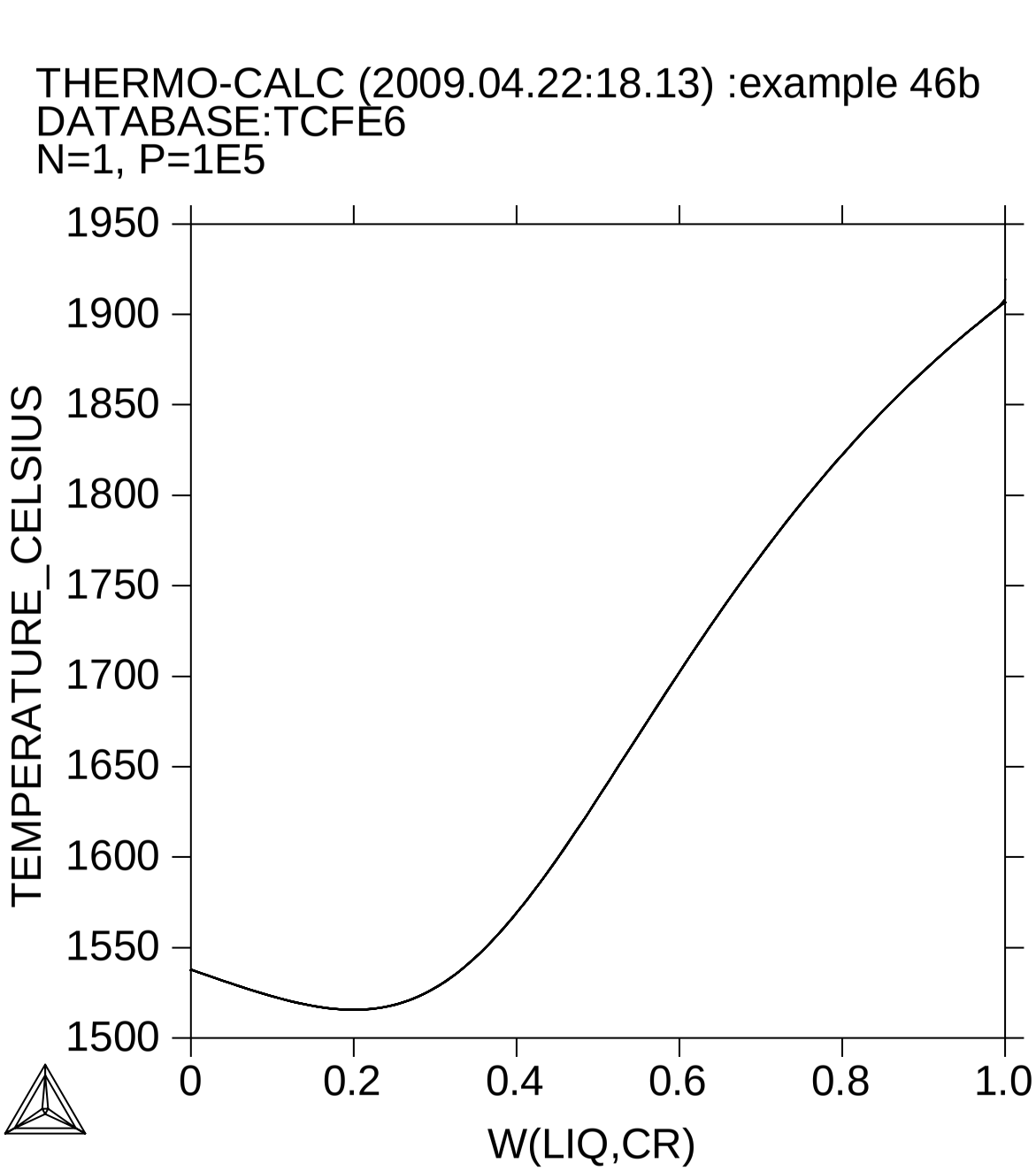
 Processing crc_liq.tab
  3.4858401E-09 <X<   1.000000
  3.3435800E-08 <Y<   1.000000
   1533.060     <Z<   4492.140
POST: ,,,,,,,
  No such command, use HELP
POST:
POST: @@ Change the diagram type to obtain a squared diagram
POST: s-d-t n,,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST:
POST: @@ Create the squared 3D-diagram
POST: cre-3d
   ... the command in full is CREATE_3D_PLOTFILE
Use current WORKSPACE (WS), TAB files or BOTH: /WS/:  BOTH
 The table must contain values for X,Y and Z axis
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    TEMP_C=T-273.15
 DEFINED TABLES
    TAB1=W(LIQUID,C), W(LIQUID,CR), TEMP_C
Table Name: tab1
Give TAB filename: /Cancel_to_finish/:  fec_liq.tab fecr_liq.tab crc_liq.tab Cancel_to
Output file: /3Dplot/:  tcex46_sqrt.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/:  .12
Y-AXIS SCALING FROM 0.0 TO YMAX /1/:  1
Z-AXIS SCALING, GIVE ZMIN /0/:  1200
Z-AXIS SCALING, GIVE ZMAX /2000/:  2200
 It is possible to combine files by:
 Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

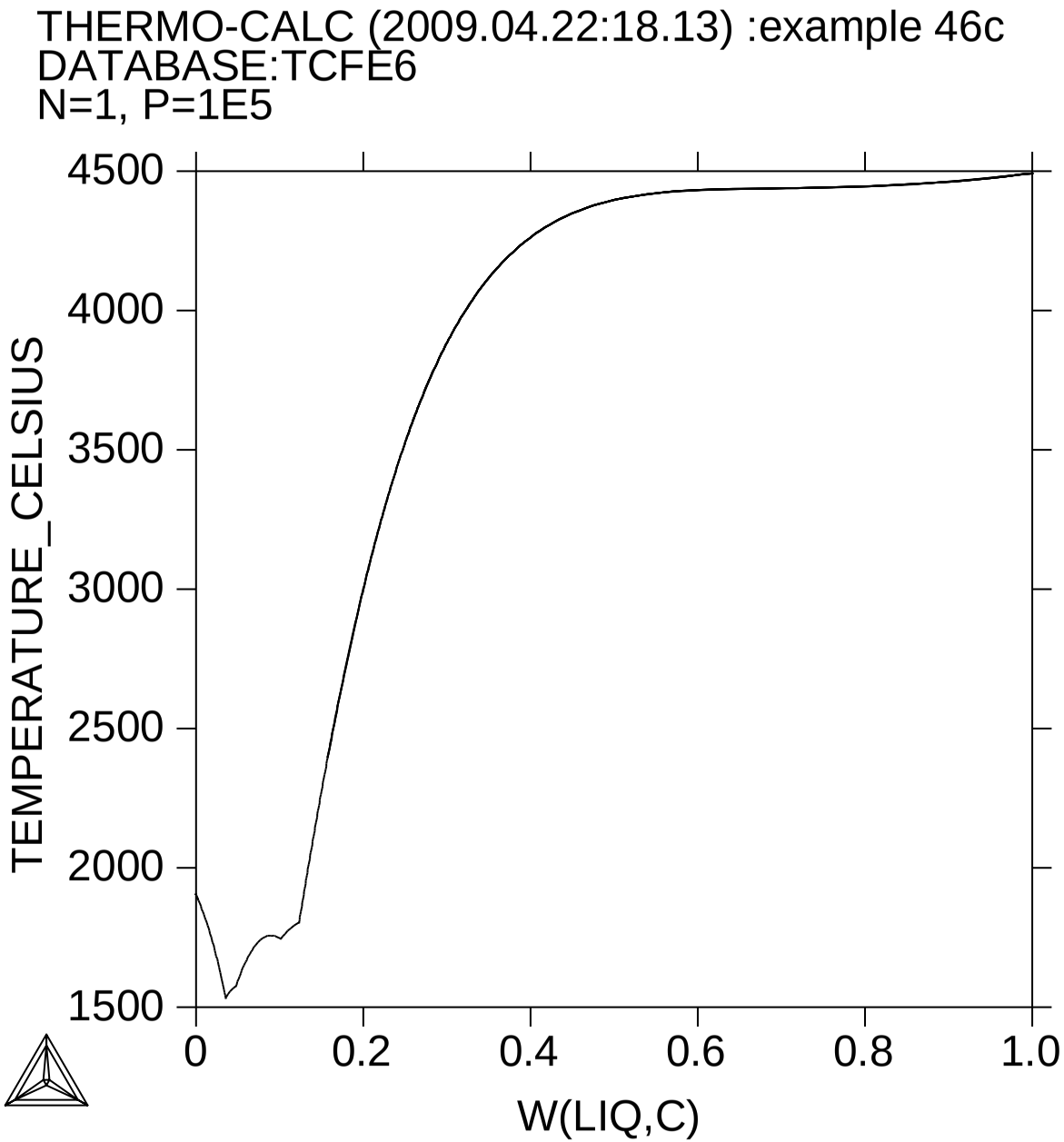
 Processing fec_liq.tab
  3.4429100E-09 <X<   1.000000
   0.000000     <Y<   0.000000
   1153.440     <Z<   4500.070

 Processing fecr_liq.tab
   0.000000     <X<   0.000000
  1.1746299E-09 <Y<   1.000000
   1515.560     <Z<   1919.760

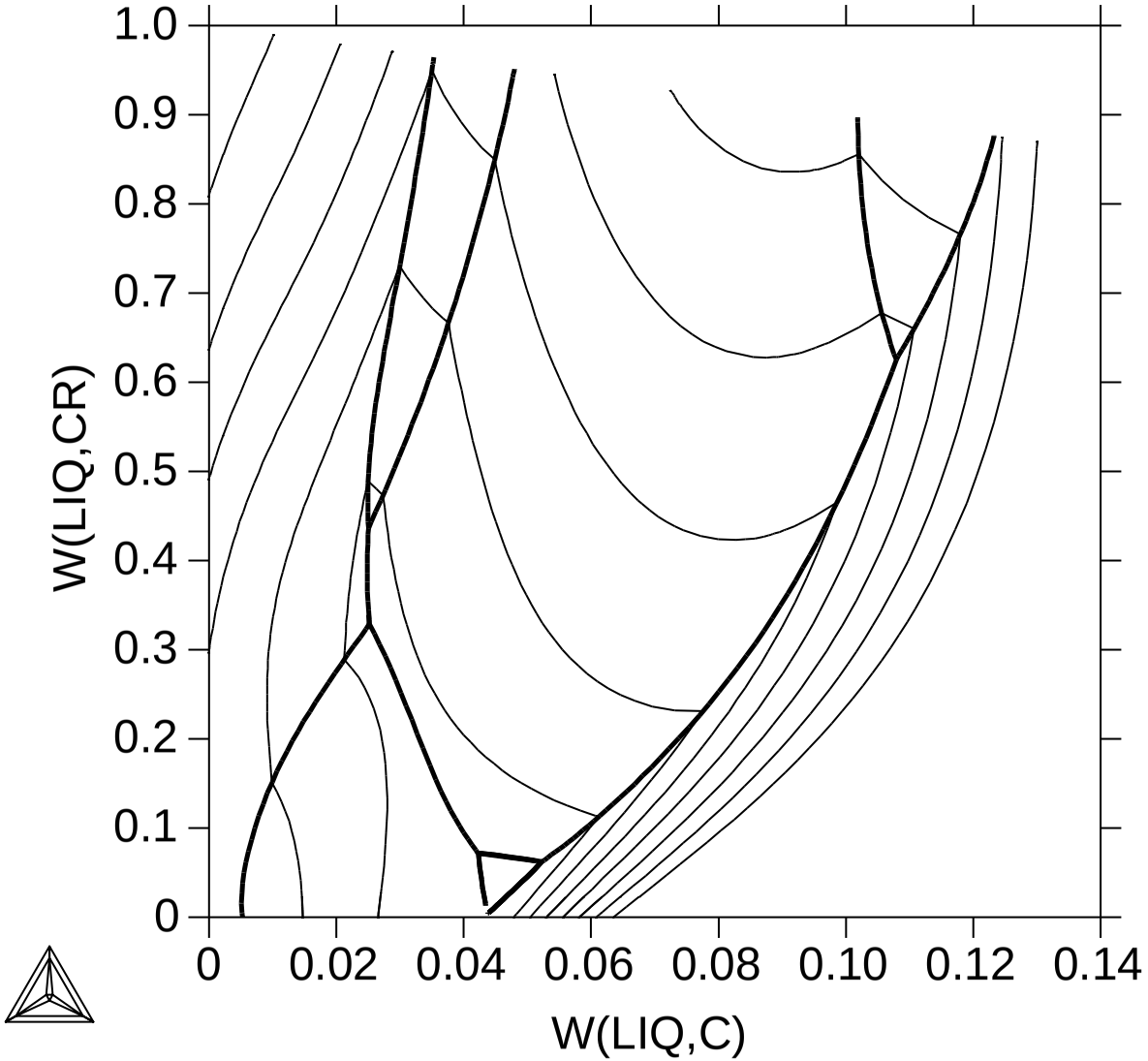
 Processing crc_liq.tab
  3.4858401E-09 <X<   1.000000
  3.3435800E-08 <Y<   1.000000
   1533.060     <Z<   4492.140
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           30  seconds
```


THERMO-CALC (2009.04.22:18.13) :example 46a
DATABASE:TCFE6
N=1, P=1E5
TEMPERATURE_CELSIUS
4500
4000
3500
3000
2500
2000
1500
1000
0
0.2
0.4
0.6
0.8
1.0
W(LIQ,C)


THERMO-CALC (2009.04.22:18.13) :example 46b
DATABASE:TCFE6
N=1, P=1E5
TEMPERATURE_CELSIUS
1950
1900
1850
1800
1750
1700
1650
1600
1550
1500
0
0.2
0.4
0.6
0.8
1.0
W(LIQ,CR)

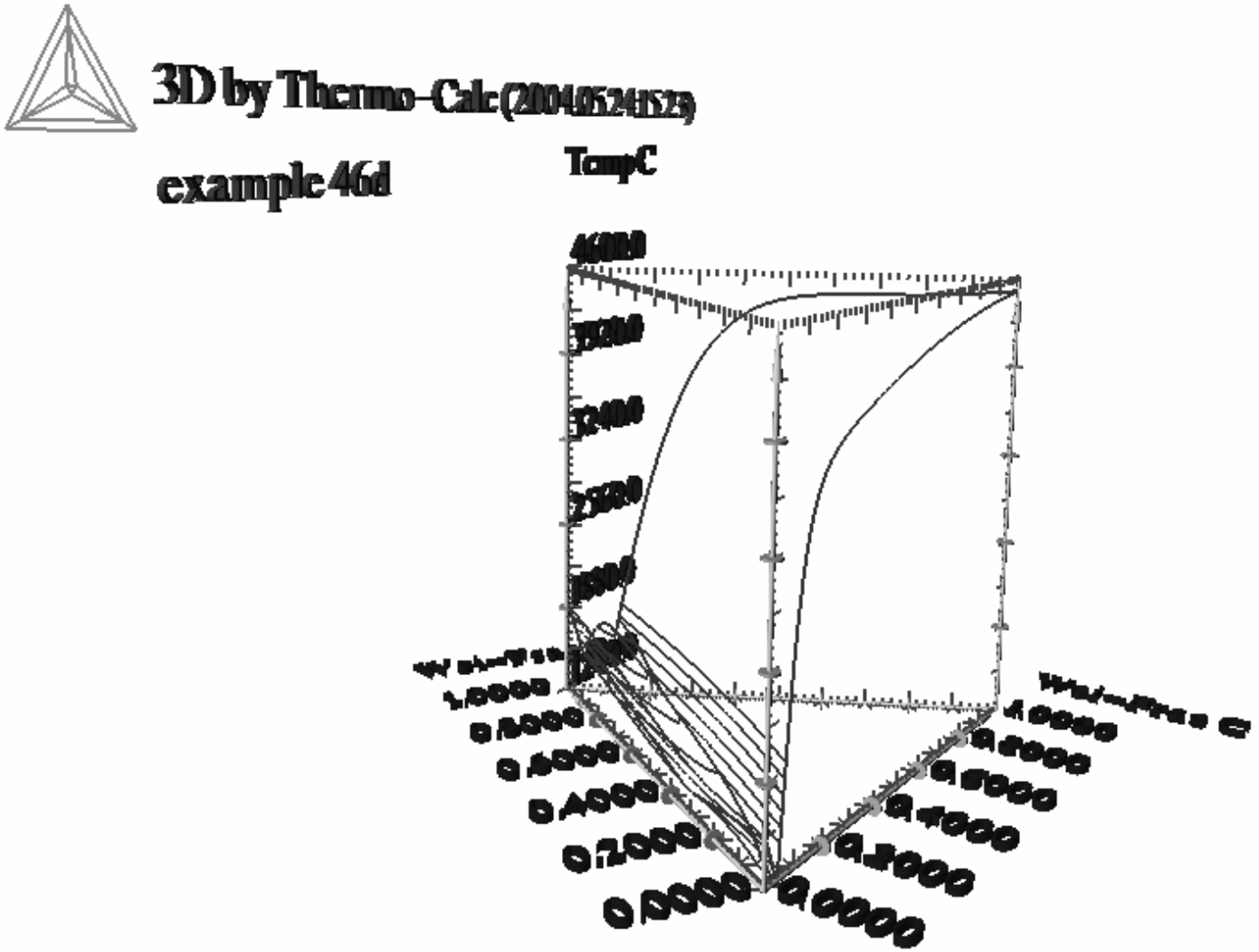

THERMO-CALC (2009.04.22:18.13) :example 46c
DATABASE:TCFE6
N=1, P=1E5
TEMPERATURE_CELSIUS
4500
4000
3500
3000
2500
2000
1500
0
0.2
0.4
0.6
0.8
1.0
W(LIQ,C)

THERMO-CALC (2009.04.22:18.13) :example 46d
DATABASE:TCFE6
N=1, P=1E5



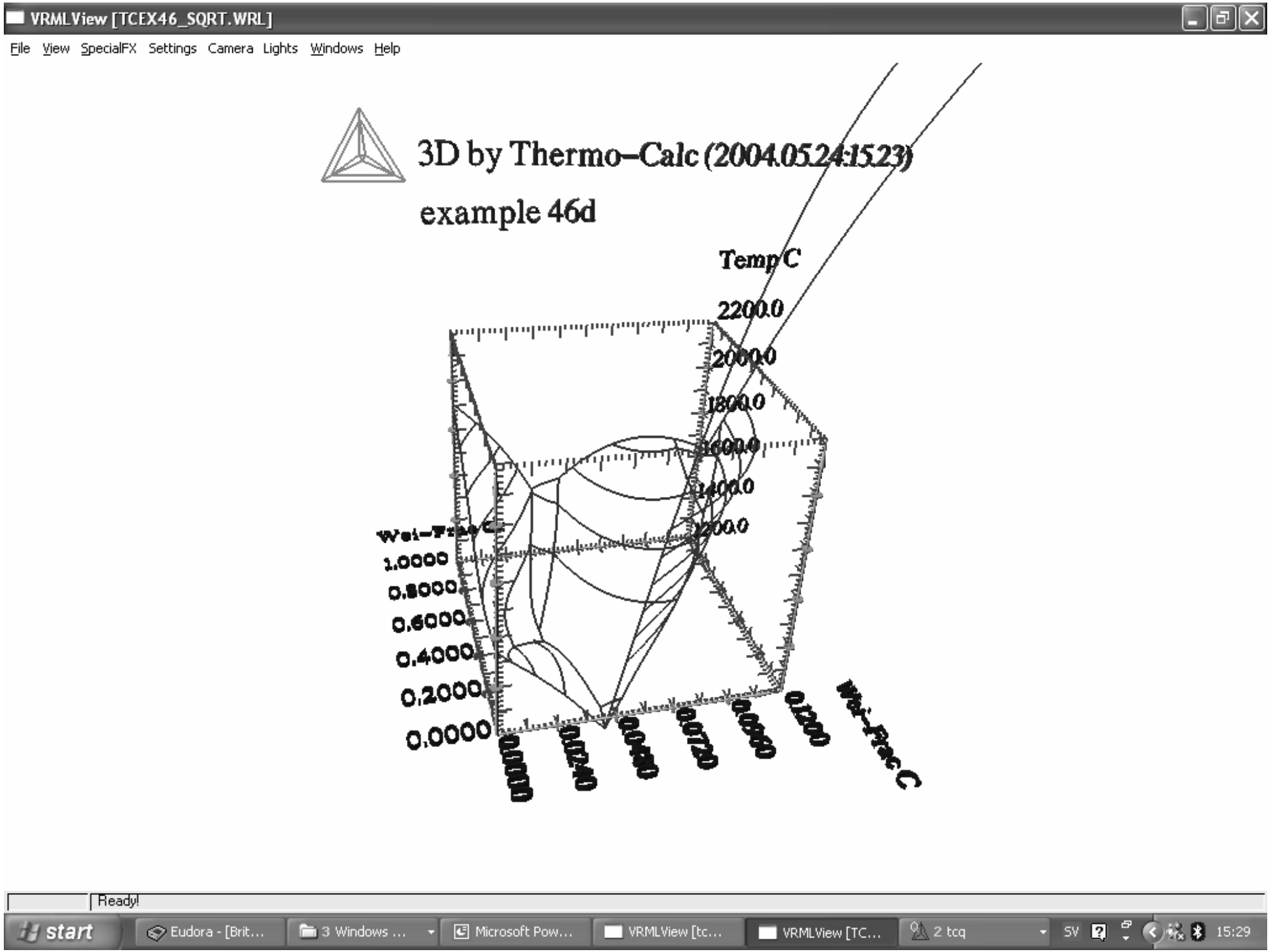
VRMLView [TCEX46_TRI.WRL]

File View SpecialFX Settings Camera Lights Windows Help



Ready!

start | Eudora - [Britt-Mari... | 3 Windows Explorer | Microsoft PowerPoi... | VRMLView [tcex47.... | VRMLView [TCEX46... | SV | 15:34


VRMLView [TCEX46_SQRT.WRL]
File View SpecialFX Settings Camera Lights Windows Help
3D by Thermo-Calc (2004.05.24:15:23)
example 46d
Temp C
2200.0
2000.0
1800.0
1600.0
1400.0
1200.0
Wei-Frac C
1.0000
0.8000
0.6000
0.4000
0.2000
0.0000
Wei-Frac C
Ready!
start
Eudora - [Brit...
3 Windows ...
Microsoft Pow...
VRMLView [tc...
VRMLView [TC...
2 tcq
SV
15:29

47

3D-Diagram
A quarternay diagram with the gamma volume in the Fe-Cr-V-C system at 1373K

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ This file calculated the gamma volume in fe-cr-v-c systeam at 110
SYS: @@ Please note that in order to view the generated file, tcex47.wrl,
SYS: @@ it's necessary to install a WRML(Wirtual Reality Modelling
SYS: @@ Language) viewer to web browser in use. WRML viwers can be
SYS: @@ downloaded witout any cost from e.g. www.parallelgraphics.com
SYS: @@ and www.sim.no
SYS:
SYS: set-log ex47
Heading:
SYS: @@ Calculate the Fe-Cr-C side of the diagram
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw PTERN
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
TDB_PTERN: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
TDB_PTERN: de-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
   DEFINED
TDB_PTERN: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  GRAPHITE                SIGMA
 CEMENTITE               M3C2                    M7C3
 M23C6                   V3C2  REJECTED
TDB_PTERN: res-ph fcc,bcc,m23,m7,cem
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  M23C6
 M7C3                    CEMENTITE  RESTORED
TDB_PTERN: get
```

```
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (19
       C-FE'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
      (1986); CR-FE'
  'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
      Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatu
  'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (198
      C-CR-FE'
 -OK-
TDB_PTERN:
TDB_PTERN: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(c)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.05
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         5731  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time    0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 1,,,,,
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
```

```
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   1.805E-01  1.817E-01
     FCC_A1#1
  ** M7C3
 *** Buffer saved on file: tcex47.POLY3
 Calculated.            5  equilibria

 Phase region boundary   2 at:   1.863E-01  1.489E-01
  ** CEMENTITE
     FCC_A1#1
  ** M7C3

 Phase region boundary   3 at:   1.613E-01  8.640E-02
  ** CEMENTITE
     FCC_A1#1
 Calculated           20  equilibria

 Phase region boundary   4 at:   1.863E-01  1.489E-01
     FCC_A1#1
  ** M7C3
 Calculated.           22  equilibria

       :
       :
       :

 Phase region boundary   6 at:   1.137E-01  3.157E-01
     FCC_A1#1
  ** M23C6
 Calculated.            5  equilibria

 Phase region boundary   7 at:   1.118E-01  3.463E-01
  ** BCC_A2
```

```
     FCC_A1#1
   ** M23C6

 Phase region boundary   8 at:   1.028E-02  1.941E-01
   ** BCC_A2
      FCC_A1#1
 Calculated           28  equilibria

 Phase region boundary   9 at:   1.805E-01  1.817E-01
      FCC_A1#1
   ** M7C3
 Calculated.           18  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex47.POLY3
 CPU time for mapping           1  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01


 Setting automatic diagram axis

POST: s-d-a x x(fcc,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 .2
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 47a
POST: plot,,,,,
POST:
POST:  @?<Hit_return_to_continue>
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc phase, in the second V content which i
POST: @@ here, and in the last column the C content of the fcc phase.
POST: e-sym tab tab1
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc,c),x(fcc,cr),ZERO
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fecrc_1373.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Fe-Cr-V side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_PTERN: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
```

```
 REINITIATING GES5 .....
TDB_PTERN: de-sys fe cr v
   ... the command in full is DEFINE_SYSTEM
 FE                    CR                    V
   DEFINED
TDB_PTERN: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L              FCC_A1                BCC_A2
 HCP_A3                SIGMA  REJECTED
TDB_PTERN: res-ph bcc,fcc
   ... the command in full is RESTORE
 BCC_A2                FCC_A1  RESTORED
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
     -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
     (1986); CR-FE'
  'W. Huang, TRITA-MAC 432 (Rev 1989,1990); FE-V'
  'J-O Andersson, CALPHAD Vol 7, (1983), p 305-315 (parameters revised 19
     due to new decription of V) TRITA 0201 (1982); FE-V'
 -OK-
TDB_PTERN:
TDB_PTERN: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.005
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         3954  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time    0  s
POLY_3:
```

```
POLY_3: s-a-v 1 x(v) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4

 Phase region boundary   1 at:   6.770E-03  9.646E-02
  ** BCC_A2
     FCC_A1
 Calculated            9  equilibria

 Phase region boundary   2 at:   6.770E-03  9.646E-02
  ** BCC_A2
     FCC_A1
 Calculated           18  equilibria

 Phase region boundary   3 at:   1.681E-02  4.915E-03
  ** BCC_A2
     FCC_A1
 Calculated           17  equilibria

 Phase region boundary   4 at:   1.681E-02  4.915E-03
  ** BCC_A2
     FCC_A1
 Calculated           27  equilibria
 *** BUFFER SAVED ON FILE: tcex47.POLY3
 CPU time for mapping           1  seconds
POLY_3:
```

```
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01


 Setting automatic diagram axis

POST: s-d-a x x(fcc,v)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .05
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 .2
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 47b
POST: pl,,,,
POST:
POST:  @?<Hit_return_to_continue>
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc phase, in the second V content which i
POST: @@ here, and in the last column the C content of the fcc phase.
POST: e-sym tab tab2
   ... the command in full is ENTER_SYMBOL
Variable(s): zero,x(fcc,cr),x(fcc,v)
&
POST: @@ Save the tabulated data on file
POST: tab tab2 fecrv_1373.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Fe-C-V side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_PTERN: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
TDB_PTERN: de-sys fe v C
   ... the command in full is DEFINE_SYSTEM
 FE                     V                      C
   DEFINED
TDB_PTERN: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L               FCC_A1                 BCC_A2
 HCP_A3                 GRAPHITE               SIGMA
 CEMENTITE              M7C3                   M23C6
 V3C2  REJECTED
TDB_PTERN: res-ph fcc,bcc,v3c2,cem,hcp
   ... the command in full is RESTORE
 FCC_A1                 BCC_A2                 V3C2
 CEMENTITE              HCP_A3  RESTORED
TDB_PTERN: get
```

```
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
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       C-FE'
  'W. Huang, TRITA-MAC 431 (1990); C-V'
  'W. Huang, TRITA-MAC 432 (Rev 1989,1990); FE-V'
  'W. Huang, TRITA-MAC 432 (1990); C-Fe-V'
  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
      Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatu
  'J-O Andersson, CALPHAD Vol 7, (1983), p 305-315 (parameters revised 19
      due to new decription of V) TRITA 0201 (1982); FE-V'
  'W. Huang, TRITA-MAC 441 (1990), Fe-Mn-V-C '
 -OK-
TDB_PTERN:
TDB_PTERN: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         5595  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time    0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(v) 0 1 .01
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 2
```

```
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3:
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Working hard
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   2.874E-03  2.701E-02
  ** BCC_A2
     FCC_A1#1
 Calculated           10  equilibria

 Phase region boundary   2 at:   2.874E-03  2.701E-02
  ** BCC_A2
     FCC_A1#1
 Calculated.            2  equilibria
 Calculated            2  equilibria

 Phase region boundary   3 at:   2.874E-03  2.701E-02
  ** BCC_A2
     FCC_A1#1
 Calculated.            2  equilibria

 Phase region boundary   4 at:   3.520E-03  2.936E-02
  ** BCC_A2
     FCC_A1#1
  ** FCC_A1#2

 Phase region boundary   5 at:   2.262E-01  2.869E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated.            8  equilibria
```

```
 Phase region boundary   6 at:   2.937E-01  2.705E-01
  ** CEMENTITE
     FCC_A1#1
  ** FCC_A1#2

 Phase region boundary   7 at:   1.682E-01  2.311E-03
  ** CEMENTITE
     FCC_A1#1
 Calculated           26  equilibria

 Phase region boundary   8 at:   3.520E-03  2.936E-02
  ** BCC_A2
     FCC_A1#1
 Calculated           15  equilibria
 *** BUFFER SAVED ON FILE: tcex47.POLY3
 CPU time for mapping           1  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01


 Setting automatic diagram axis

POST: s-d-a x x(fcc,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc,v)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 .1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 47c
POST: plot,,,,
POST:
POST:  @?<Hit_return_to_continue>
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc phase, in the second V content which i
POST: @@ here, and in the last column the C content of the fcc phase.
POST: e-sym tab tab3
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc,c),zero,x(fcc,v)
&
POST: @@ Save the tabulated data on file
POST: tab tab3 fevc_1373.tab
   ... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Cr-V-C side of the diagram
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_PTERN: rej-sys
   ... the command in full is REJECT
```

```
 VA  DEFINED
 REINITIATING GES5 .....
TDB_PTERN: de-sys cr v C
   ... the command in full is DEFINE_SYSTEM
 CR                    V                     C
   DEFINED
TDB_PTERN: @@No fcc phase in this system we skip this calc
TDB_PTERN:
TDB_PTERN: @@ Next calculate a projection of the Fe-Cr-V-C system
TDB_PTERN: go data
   ... the command in full is GOTO_MODULE
 *** You have not executed the GET_DATA command

TDB_PTERN: rej-sys
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES5 .....
TDB_PTERN: de-sys fe cr v C
   ... the command in full is DEFINE_SYSTEM
 FE                    CR                    V
 C  DEFINED
TDB_PTERN: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L              FCC_A1                BCC_A2
 HCP_A3                GRAPHITE              SIGMA
 CEMENTITE             M3C2                  M7C3
 M23C6                 V3C2  REJECTED
TDB_PTERN: res-ph fcc,bcc,hcp,m23,fcc,bcc,m23,m7,cem,v3c2
   ... the command in full is RESTORE
 FCC_A1                BCC_A2                HCP_A3
 M23C6                 M7C3                  CEMENTITE
 V3C2  RESTORED
TDB_PTERN: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (19
       C-FE'
```

```
  'W. Huang, TRITA-MAC 431 (1990); C-V'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
     (1986); CR-FE'
  'W. Huang, TRITA-MAC 432 (Rev 1989,1990); FE-V'
  'W. Huang, TRITA-MAC 432 (1990); C-Fe-V'
  'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
     Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatu
  'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (198
     C-CR-FE'
  'J-O Andersson, CALPHAD Vol 7, (1983), p 305-315 (parameters revised 19
     due to new decription of V) TRITA 0201 (1982); FE-V'
  'W. Huang, TRITA-MAC 441 (1990), Fe-Mn-V-C '
 -OK-
TDB_PTERN:
TDB_PTERN: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc,cr)=.02
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         6863  grid points in            0  s
    30 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .005
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(v) 0 1 .005
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc,cr)=.04
   ... the command in full is SET_CONDITION
POLY_3: c-e
```

```
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    15 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc,cr)=.06
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    15 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc,cr)=.08
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    22 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc,cr)=.10
   ... the command in full is SET_CONDITION
```

```
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    15 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc,cr)=.12
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    15 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc,cr)=.14
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    15 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.005
   ... the command in full is SET_CONDITION
POLY_3: se-co x(fcc,cr)=.16
   ... the command in full is SET_CONDITION
```

```
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    34 ITS,  CPU TIME USED   0 SECONDS
POLY_3:
POLY_3: add-in 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
      :
      :
      :
 Generating start point  31
 Generating start point  32

 Phase region boundary   1 at:   5.000E-02  5.627E-03
     FCC_A1#1
  ** FCC_A1#2
 Calculated.           11  equilibria
```

```
 Phase region boundary   2 at:   6.828E-03  2.436E-02
  ** BCC_A2
     FCC_A1#1
  ** FCC_A1#2

 Phase region boundary   3 at:   6.828E-03  2.436E-02
     BCC_A2
     FCC_A1#1
  ** FCC_A1#2
 Calculated.            4  equilibria
 Terminating at known equilibrium
       :
       :
       :
 Phase region boundary 106 at:   5.000E-02  1.414E-02
     FCC_A1#1
  ** FCC_A1#2
     M23C6
 Calculated.           33  equilibria
 Terminating at known equilibrium

 Phase region boundary 107 at:   1.514E-01  5.000E-03
     FCC_A1#1
  ** FCC_A1#2
     M23C6
 Calculated.           13  equilibria
 Terminating at known equilibrium

 Phase region boundary 108 at:   1.514E-01  5.000E-03
     FCC_A1#1
  ** FCC_A1#2
     M23C6
 Calculated.           27  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex47.POLY3
 CPU time for mapping          26  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01


 Setting automatic diagram axis

POST: s-d-a x x(fcc,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc,v)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z x(fcc,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-a-t-s y y
   ... the command in full is SET_AXIS_TEXT_STATUS
```

```
POST: s-a-t-s x y
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s z y
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-s-s x n 0 0.1
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 0.05
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s z n 0 0.2
   ... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 47d
POST: plot,,,,
POST:
POST:
POST:  @?<Hit_return_to_continue>
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc phase, in the second V content which i
POST: @@ here, and in the last column the C content of the fcc phase.
POST: e-sym tab tab4
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc,c),x(fcc,cr),x(fcc,v)
&
POST: @@ Save the tabulated data on file
POST: tab tab4 fecrvc_1373.tab
   ... the command in full is TABULATE
POST:
POST:
POST: back
POLY_3: rei,,,,
   ... the command in full is REINITIATE_MODULE
POLY_3:
POLY_3: s-c t=1373
   ... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
   ... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.01
   ... the command in full is SET_CONDITION
POLY_3: se-co x(v)=.001
   ... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.01
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         6863  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .001
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(v) 0 1 .001
```

```
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 1,,,
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(cr)=.05
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1,,,
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(cr)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Using already calculated grid
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: add-in 1,,,
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  present
Phase name /NONE/:  fcc
POLY_3: save tcex47 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
```

```
 Phase region boundary   1 at:   8.090E-02  1.000E-03
  ** CEMENTITE
     FCC_A1#1
 Calculated           22  equilibria

 Phase region boundary   2 at:   8.090E-02  1.000E-03
  ** CEMENTITE
     FCC_A1#1
 Calculated           10  equilibria

 Phase region boundary   3 at:   8.090E-02  1.000E-03
  ** CEMENTITE
     FCC_A1#1
 Calculated.            5  equilibria
   :
   :
   :
 Phase region boundary  60 at:   1.314E-02  2.071E-02
  ** BCC_A2
     FCC_A1#1
 Calculated           42  equilibria

 Phase region boundary  61 at:   1.314E-02  2.071E-02
  ** BCC_A2
     FCC_A1#1
     FCC_A1#2
 Calculated.          329  equilibria
 Terminating at known equilibrium

 Phase region boundary  62 at:   3.632E-02  9.733E-03
     FCC_A1#1
  ** FCC_A1#2
     M7C3
 Calculated.          105  equilibria
 Terminating at known equilibrium

 Phase region boundary  63 at:   3.632E-02  9.733E-03
     FCC_A1#1
  ** M7C3
 Calculated           27  equilibria
 *** BUFFER SAVED ON FILE: tcex47.POLY3
 CPU time for mapping          33  seconds
POLY_3:
POLY_3: post

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01


 Setting automatic diagram axis

POST:
POST: se-d-t n y,,,
   ... the command in full is SET_DIAGRAM_TYPE
```

```
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc phase, in the second V content which i
POST: @@ here, and in the last column the C content of the fcc phase.
POST: e-sym tab tab5
   ... the command in full is ENTER_SYMBOL
Variable(s): x(fcc,c),x(fcc,cr),x(fcc,v)
&
POST: se-tit
   ... the command in full is SET_TITLE
TITLE : Fe-Cr-V-C system
POST: s-d-a x x(fcc,c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc,cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z x(fcc,v)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-a-t-s x n X(C)
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s y n X(Cr)
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s z n X(V)
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data
POST: @@ from the different tables created and saved. This is accomplishe
POST: @@ using the command "CREATE_3D_DIAGRAM". Also define the scaling
POST: @@ to be used in the 3D-diagram.
POST: cre BOTH tab5
   ... the command in full is CREATE_3D_PLOTFILE
 The table must contain values for X,Y and Z axis
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    TEMP_C=T-273.15
 DEFINED TABLES
    TAB5=X(FCC_A1#1,C), X(FCC_A1#1,CR), X(FCC_A1#1,V)
Give TAB filename: /Cancel_to_finish/:  fecrc_1373.tab fecrv_1373.tab fev
Output file: /3Dplot/:  tcex47.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/:  .1
Y-AXIS SCALING FROM 0.0 TO YMAX /1/:  .2
 TETRAHEDRON DIAGRAM, ZMIN SET 0.0
Z-AXIS SCALING, GIVE ZMAX /2000/:  .1
 TETRAHEDRON DIAGRAM, XMAX AND YMAX SET EQUAL

 It is possible to combine files by:
 Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

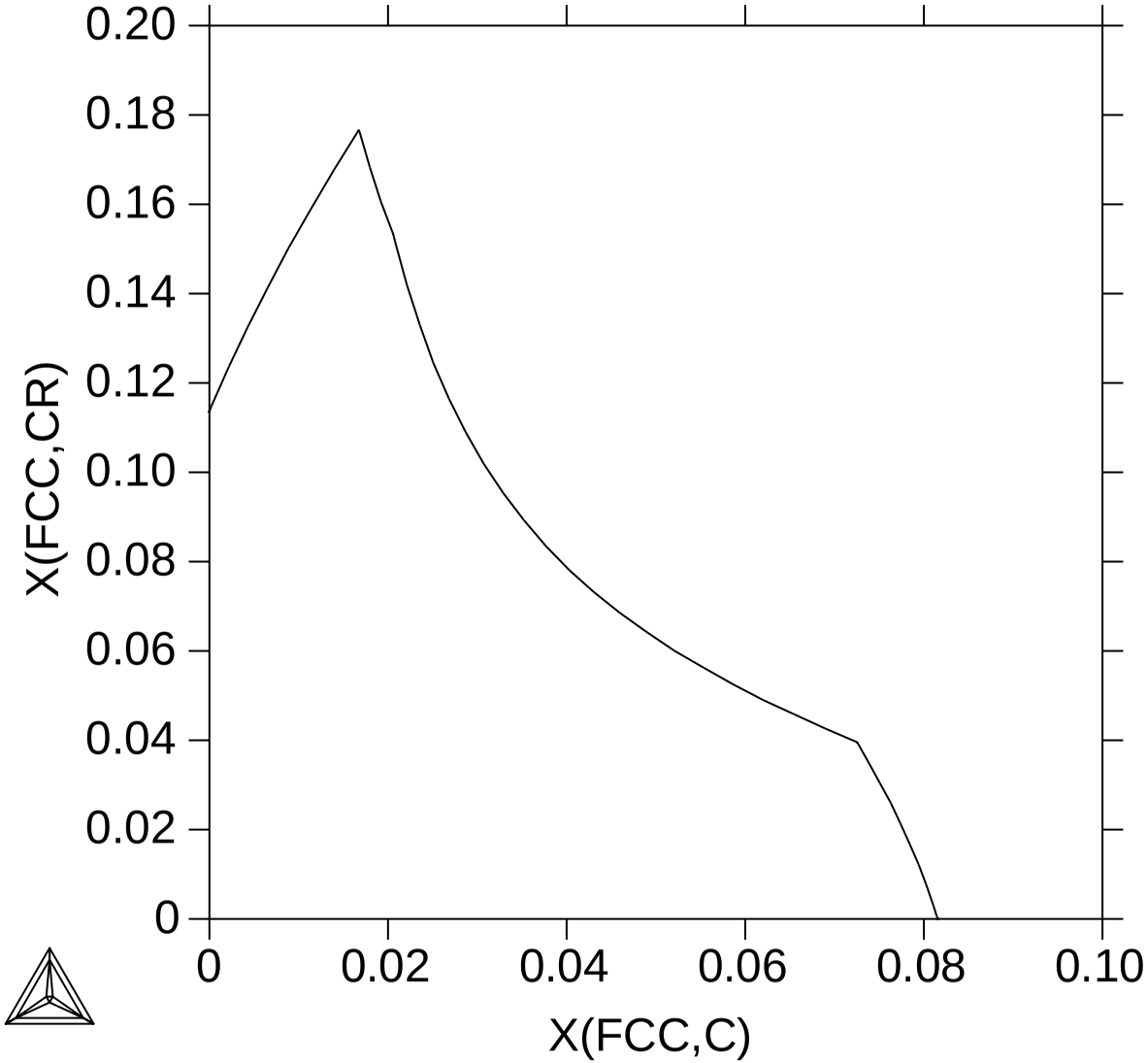
 Processing fecrc_1373.tab
  5.6316800E-09 <X<  8.1581101E-02
  2.5539300E-09 <Y<  0.1766470
   0.000000     <Z<   0.000000
```

```
 Processing fecrv_1373.tab
   0.000000     <X<   0.000000
  6.5356600E-09 <Y<  0.1136370
  1.0000000E-12 <Z<  1.3302700E-02

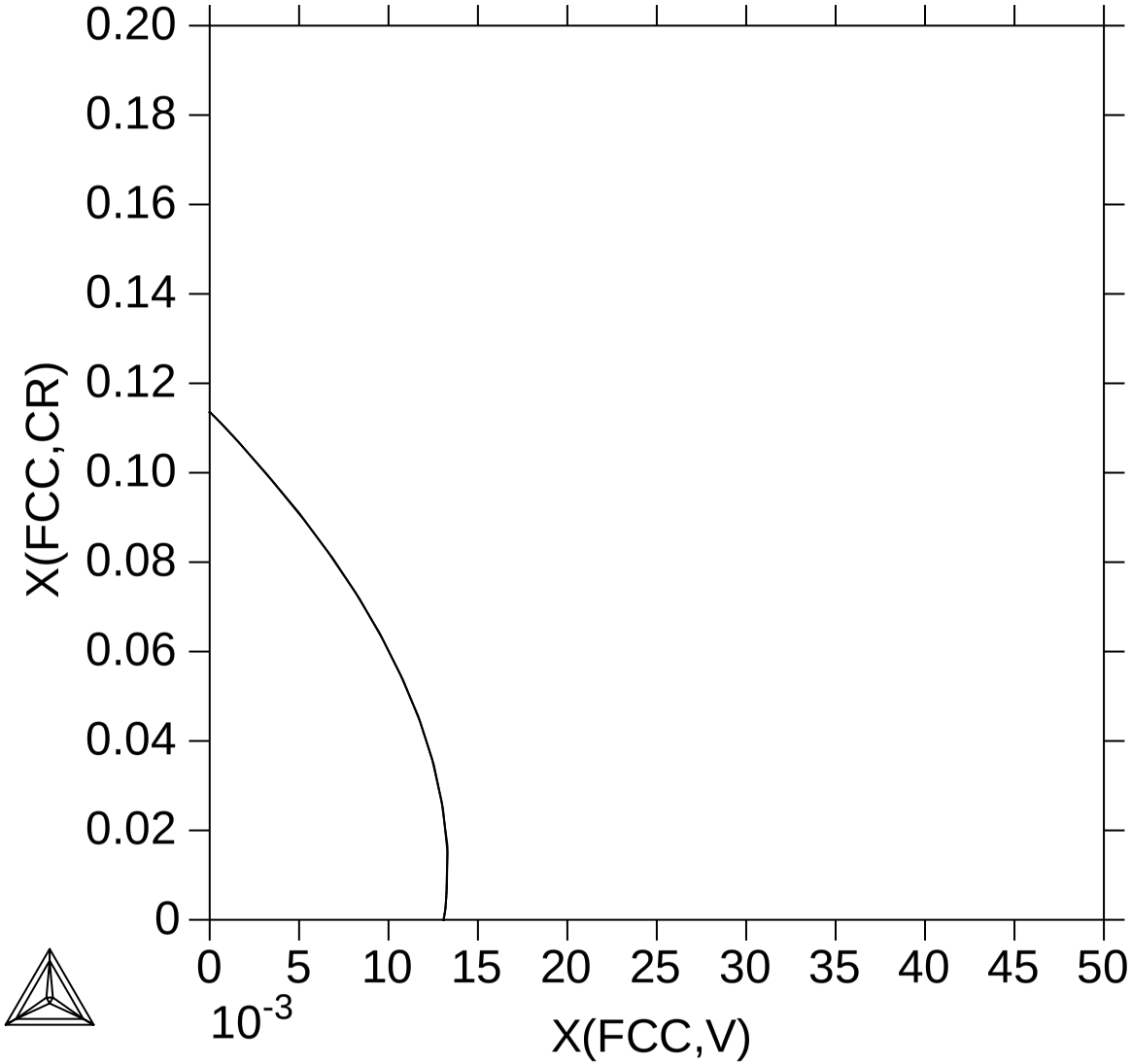
 Processing fevc_1373.tab
  1.2718900E-08 <X<  8.6466499E-02
   0.000000     <Y<   0.000000
  9.1854801E-13 <Z<  2.3953101E-02

 Processing fecrvc_1373.tab
  5.2219101E-10 <X<  8.3313398E-02
  2.0000000E-02 <Y<  0.1600000
  9.2228905E-13 <Z<  2.4364401E-02
POST:
POST:
POST:
POST: se-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           70  seconds
```

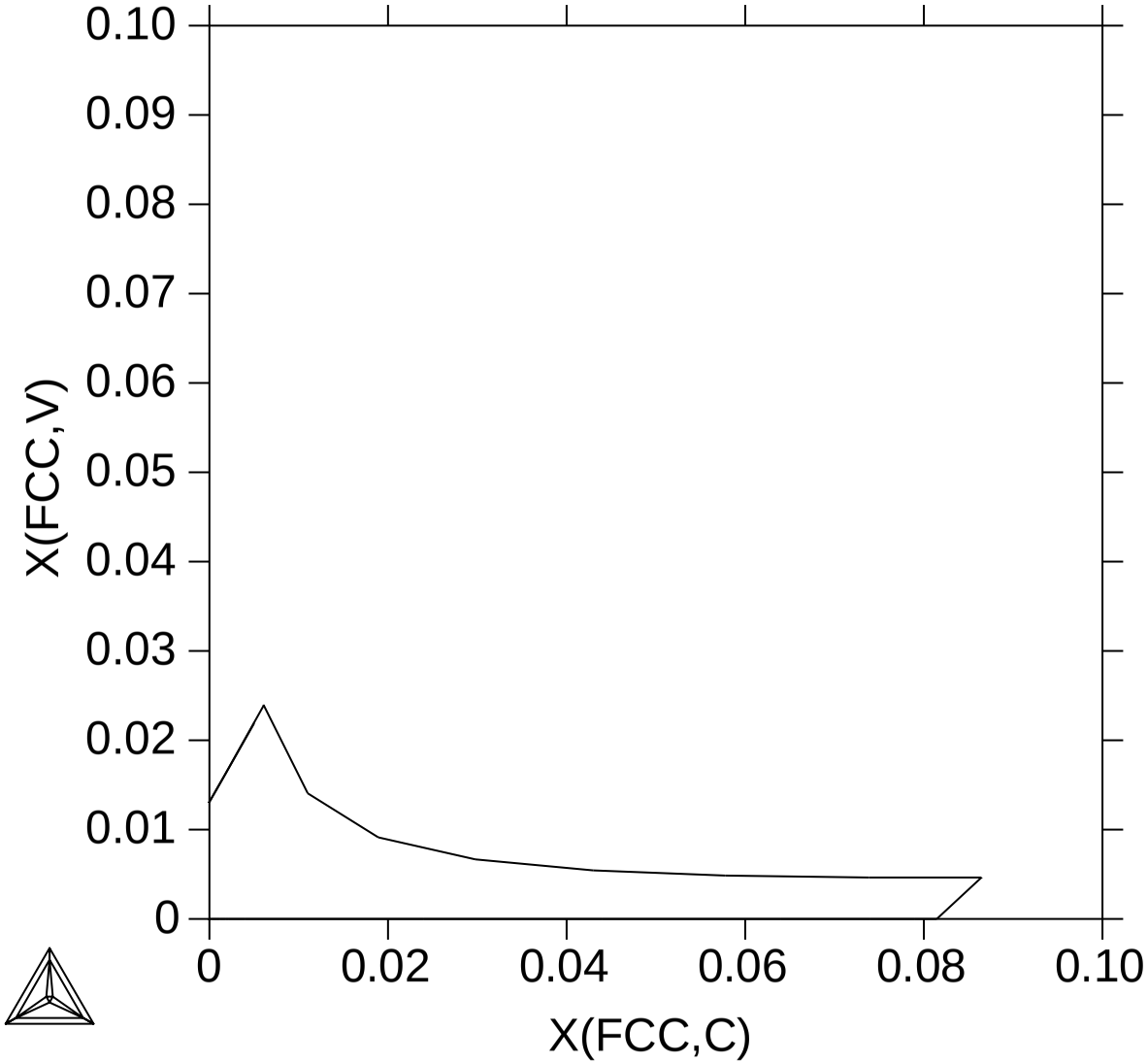
THERMO-CALC (2009.04.27:14.38) :example 47a
DATABASE:PTERN
T=1373, N=1, P=1E5;

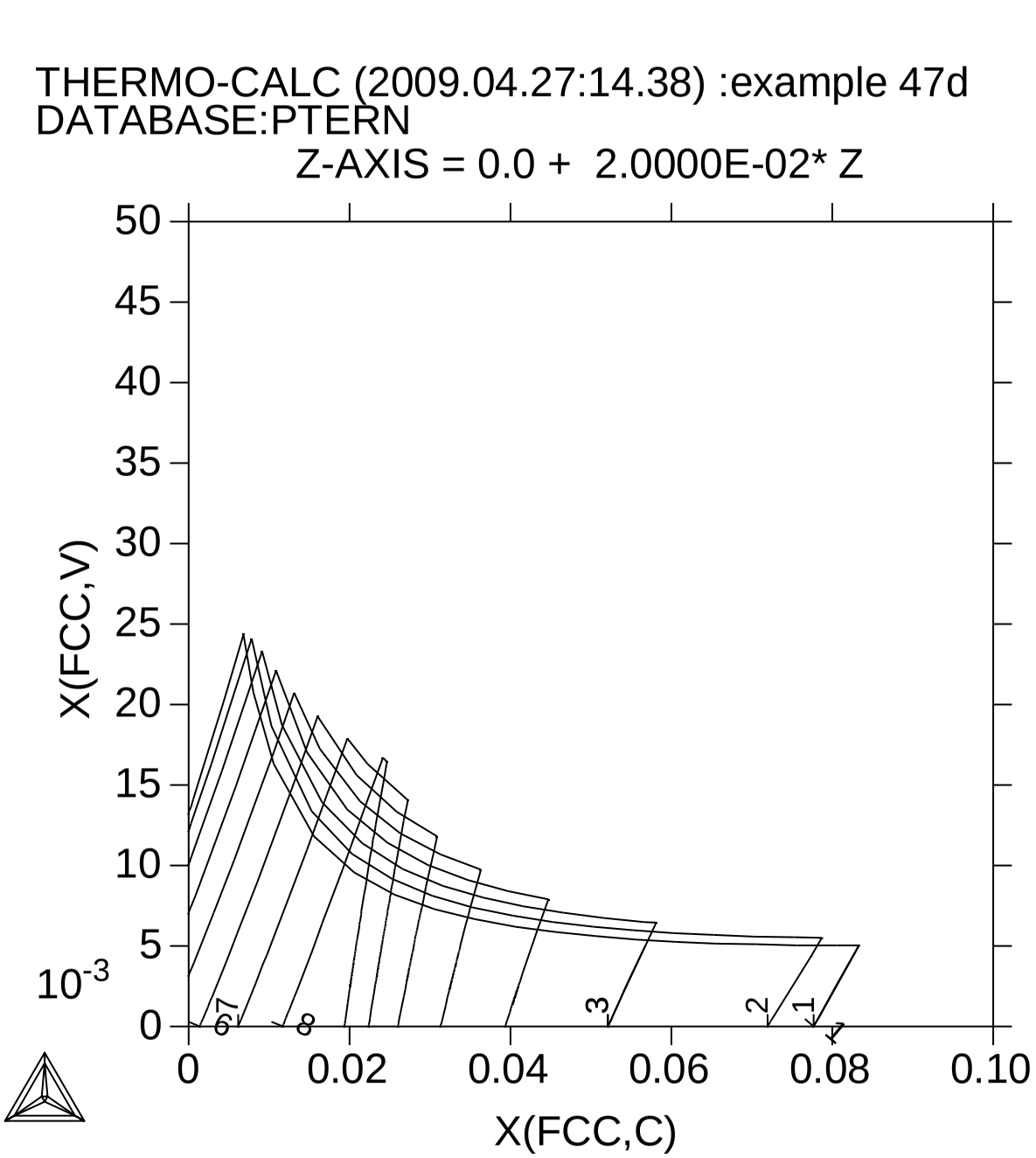


THERMO-CALC (2009.04.27:14.38) :example 47b
DATABASE:PTERN
T=1373, N=1, P=1E5;



THERMO-CALC (2009.04.27:14.38) :example 47c
DATABASE:PTERN
T=1373, N=1, P=1E5;



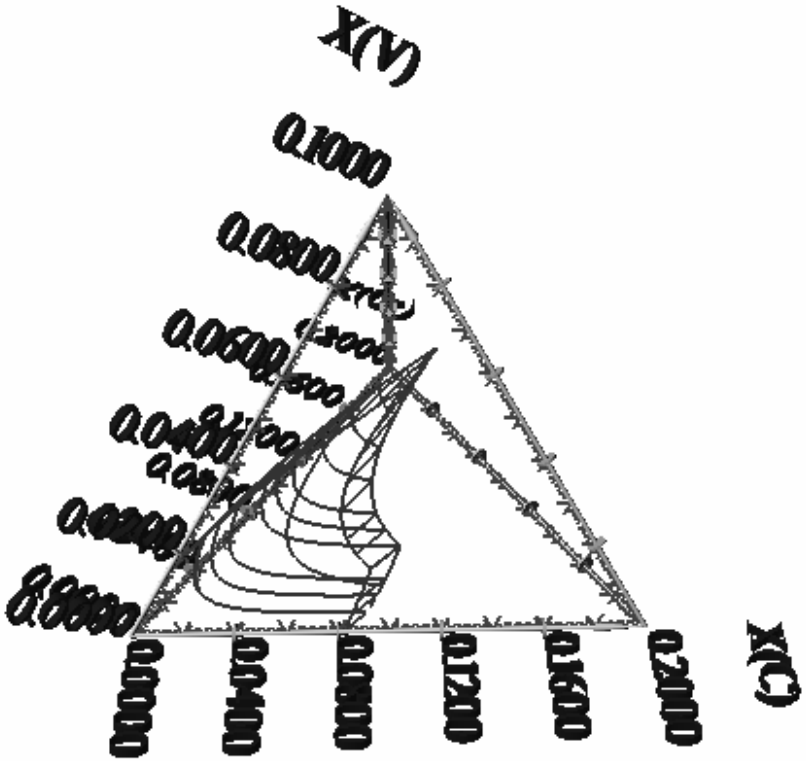

THERMO-CALC (2009.04.27:14.38) :example 47d
DATABASE:PTERN
Z-AXIS = 0.0 + 2.0000E-02* Z
50
45
40
35
30
25
20
15
10
5
0
10-3
X(FCC,V)
0
0.02
0.04
0.06
0.08
0.10
X(FCC,C)
1
2
3
4
5
6
7
8

VRMLView [tcex47.wrl]

File View SpecialFX Settings Camera Lights Windows Help

3D by Thermo-Calc *(2004.05.24:17.15)*

Fe-Cr-V-C system



Ready!

start | Eudora - [Brit... | tcex47 | Temp | qing on 'Samb... | Microsoft Pow... | VRMLView [tc... | SV | 15:18

48

Scheil Simulation with Interstitial Back Diffusion

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@  Scheil solidification with C back diffusion (ScheiC) in solid phases
SYS: @@                              and
SYS: @@  comparison with simple Scheil and equilibrium calculations
SYS: @@
SYS: set-log ex48,,,
SYS: @@ use system command delete old exp files if any
SYS: @@ for unix
SYS: @rm *.exp
SYS: @@ for pc
SYS: @@del *.exp
SYS: @@
SYS: @@ first do ScheiC by assigning C as fast diffuse element
SYS: @@ plot solidification and microsegregation diagram and save them
SYS: @@ to files
SYS: @@
SYS: go sc
   ... the command in full is GOTO_MODULE

         SCHEIL_GULLIVER SIMULATION MODULE VERSION 4.0

 ..........................................................
 .                                                        .
 .        1. Start new simulation                         .
 .        2. Open old file and plot diagram               .
 .        3. Open old file and make another simulation    .
 .                                                        .
 ..........................................................

Select option /1/:  1
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
Database /TCFE6/:  ptern
 Current database: TCS Public Ternary Alloys TDB v1

 VA  DEFINED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:  Y
1st alloying element: c 1
2nd alloying element: cr 10
Next alloying element:
Temperature (C) /2000/:  2000
 VA  DEFINED
 REINITIATING GES5 .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED

 This database has following phases for the defined system

 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  GRAPHITE                SIGMA
 CEMENTITE               M3C2                    M7C3
 M23C6                   V3C2

Reject phase(s) /NONE/:  NONE
Restore phase(s): /NONE/:  NONE
 ..................................................
```

```
   The following phases are retained in this system:

 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  GRAPHITE                SIGMA
 CEMENTITE               M3C2                    M7C3
 M23C6                   V3C2

 ..................................................

OK? /Y/:  Y
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317
      -425, also in NPL Report DMA(A)195 Rev. August 1990'
  'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
  'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267 TRITA 0237 (1984);
       C-FE'
  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92 TRITA 0270
      (1986); CR-FE'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database, v1.2;
      Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters at high temperatures.'
  'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636 TRITA 0207 (1986);
      C-CR-FE'
  'W. Huang, TRITA-MAC 441 (1990), Fe-Mn-V-C '
 -OK-
Should any phase have a miscibility gap check? /N/:  N
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
     Calculated liquidus temperature is 1441.00(C)
     Please enter simulation conditions !

Temperature step (C) /1/:  1
Default stop point? /Y/:  Y
Fast diffusing components: /NONE/:  C
Allow BCC -> FCC ? /N/:  N
Buffer-saving file name /scheil/:  tcex48a
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
   ... the command in full is ADVANCED_OPTIONS
   ... the command in full is STEP_WITH_OPTIONS

 Phase Region from    1714.15     for:
     LIQUID
 Calculated     4 equilibria

 Phase Region from    1713.15     for:
     LIQUID
     FCC_A1#2
 Calculated   111 equilibria

 Phase Region from    1605.28     for:
     FCC_A1#2
 *** Buffer saved on file: tcex48a.POLY3

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis
```

```
  ... the command in full is ENTER_SYMBOL
  ... the command in full is MAKE_EXPERIMENTAL_DATAFI
An EXP file tcex48a_EQ.EXP
has been created to store the equilibrium            solidification results.
  ... the command in full is READ_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

  ... the command in full is STEP_WITH_OPTIONS

Phase Region from    1715.15     for:
    LIQUID

Phase Region from    1712.65     for:
    LIQUID
    FCC_A1#1
      1712.6500          0.9879          0.0121             0.0000
      1712.1500          0.9760          0.0240          -166.7876
      1711.6500          0.9644          0.0356          -330.9532
      1711.1500          0.9528          0.0472          -492.5505
      1710.6500          0.9415          0.0585          -651.6327
      1710.1500          0.9303          0.0697          -808.2513
      1709.6500          0.9193          0.0807          -962.4567
      1709.1500          0.9085          0.0915         -1114.2977
      1708.6500          0.8978          0.1022         -1263.8219
      1708.1500          0.8873          0.1127         -1411.0755
      1707.6500          0.8769          0.1231         -1556.1037
      1707.1500          0.8667          0.1333         -1698.9502
      1706.6500          0.8566          0.1434         -1839.6579
      1706.1500          0.8467          0.1533         -1978.2683
      1705.6500          0.8369          0.1631         -2114.8220
      1705.1500          0.8272          0.1728         -2249.3585
      1704.6500          0.8177          0.1823         -2381.9162
      1704.1500          0.8084          0.1916         -2512.5327
      1703.6500          0.7991          0.2009         -2641.2444
      1703.1500          0.7900          0.2100         -2768.0871
      1702.6500          0.7810          0.2190         -2893.0955
      1702.1500          0.7721          0.2279         -3016.3036
      1701.6500          0.7634          0.2366         -3137.7442
      1701.1500          0.7548          0.2452         -3257.4498
      1700.6500          0.7463          0.2537         -3375.4518
      1700.1500          0.7379          0.2621         -3491.7808
      1699.6500          0.7296          0.2704         -3606.4668
      1699.1500          0.7214          0.2786         -3719.5392
      1698.6500          0.7134          0.2866         -3831.0264
      1698.1500          0.7054          0.2946         -3940.9563
      1697.6500          0.6976          0.3024         -4049.3561
      1697.1500          0.6898          0.3102         -4156.2526
      1696.6500          0.6822          0.3178         -4261.6715
      1696.1500          0.6747          0.3253         -4365.6383
      1695.6500          0.6672          0.3328         -4468.1779
      1695.1500          0.6599          0.3401         -4569.3143
      1694.6500          0.6526          0.3474         -4669.0714
      1694.1500          0.6455          0.3545         -4767.4723
      1693.6500          0.6384          0.3616         -4864.5395
      1693.1500          0.6315          0.3685         -4960.2953
      1692.6500          0.6246          0.3754         -5054.7612
      1692.1500          0.6178          0.3822         -5147.9584
      1691.1500          0.6054          0.3946         -5320.5051
      1690.6500          0.5981          0.4019         -5418.8100
      1689.6500          0.5861          0.4139         -5585.2479
      1689.1500          0.5789          0.4211         -5680.3442
      1688.1500          0.5674          0.4326         -5839.8643
      1687.6500          0.5605          0.4395         -5931.7054
      1686.6500          0.5495          0.4505         -6084.6278
      1686.1500          0.5428          0.4572         -6173.3349
      1685.1500          0.5322          0.4678         -6319.9890
      1684.6500          0.5257          0.4743         -6405.6762
      1683.6500          0.5155          0.4845         -6546.3703
      1683.1500          0.5092          0.4908         -6629.1466
      1682.1500          0.4994          0.5006         -6764.1692
      1681.6500          0.4933          0.5067         -6844.1387
```

1680.6500	0.4839	0.5161	-6973.7605
1680.1500	0.4780	0.5220	-7051.0223
1679.1500	0.4689	0.5311	-7175.4977
1678.6500	0.4632	0.5368	-7250.1467
1677.6500	0.4545	0.5455	-7369.7146
1676.6500	0.4454	0.5546	-7493.1770
1676.1500	0.4398	0.5602	-7565.2547
1675.1500	0.4316	0.5684	-7677.5113
1674.1500	0.4229	0.5771	-7793.3580
1673.1500	0.4144	0.5856	-7907.8355
1672.6500	0.4091	0.5909	-7974.9276
1671.6500	0.4016	0.5984	-8077.5030
1670.6500	0.3937	0.6063	-8183.4838
1669.6500	0.3858	0.6142	-8288.3620
1668.6500	0.3781	0.6219	-8391.0642
1667.6500	0.3705	0.6295	-8491.3684
1666.6500	0.3631	0.6369	-8589.2653
1665.6500	0.3559	0.6441	-8684.7987
1664.6500	0.3488	0.6512	-8778.0245
1663.6500	0.3419	0.6581	-8869.0009
1662.6500	0.3351	0.6649	-8957.7851
1661.6500	0.3286	0.6714	-9044.4327
1660.6500	0.3221	0.6779	-9128.9979
1659.6500	0.3158	0.6842	-9211.5334
1658.6500	0.3096	0.6904	-9292.0901
1657.6500	0.3036	0.6964	-9370.7176
1656.6500	0.2977	0.7023	-9447.4641
1655.6500	0.2920	0.7080	-9522.3764
1654.6500	0.2864	0.7136	-9595.5000
1653.6500	0.2809	0.7191	-9666.8791
1652.6500	0.2755	0.7245	-9736.5569
1651.6500	0.2702	0.7298	-9804.5752
1650.6500	0.2651	0.7349	-9870.9749
1649.6500	0.2601	0.7399	-9935.7955
1648.6500	0.2552	0.7448	-9999.0759
1647.6500	0.2504	0.7496	-10060.8538
1646.6500	0.2457	0.7543	-10121.1658
1645.6500	0.2411	0.7589	-10180.0478
1644.6500	0.2367	0.7633	-10237.5347
1643.6500	0.2323	0.7677	-10293.6605
1642.6500	0.2280	0.7720	-10348.4585
1641.6500	0.2238	0.7762	-10401.9610
1640.6500	0.2197	0.7803	-10454.1998
1639.6500	0.2158	0.7842	-10505.2055
1638.6500	0.2119	0.7881	-10555.0083
1637.6500	0.2080	0.7920	-10603.6377
1636.6500	0.2043	0.7957	-10651.1223
1635.6500	0.2007	0.7993	-10697.4901
1634.6500	0.1971	0.8029	-10742.7685
1633.6500	0.1936	0.8064	-10786.9842
1632.6500	0.1902	0.8098	-10830.1633
1631.6500	0.1869	0.8131	-10872.3312
1630.6500	0.1837	0.8163	-10913.5129
1629.6500	0.1805	0.8195	-10953.7326
1628.6500	0.1774	0.8226	-10993.0140
1627.6500	0.1743	0.8257	-11031.3804
1626.6500	0.1714	0.8286	-11068.8543
1625.6500	0.1685	0.8315	-11105.4579
1624.6500	0.1657	0.8343	-11141.2128
1623.6500	0.1629	0.8371	-11176.1400
1622.6500	0.1602	0.8398	-11210.2600
1621.6500	0.1575	0.8425	-11243.5931
1620.6500	0.1550	0.8450	-11276.1588
1619.6500	0.1524	0.8476	-11307.9763
1618.6500	0.1500	0.8500	-11339.0643
1617.6500	0.1476	0.8524	-11369.4410
1616.6500	0.1452	0.8548	-11399.1243
1615.6500	0.1429	0.8571	-11428.1315
1614.6500	0.1406	0.8594	-11456.4797
1613.6500	0.1384	0.8616	-11484.1853
1612.6500	0.1363	0.8637	-11511.2646
1611.6500	0.1342	0.8658	-11537.7333
1610.6500	0.1321	0.8679	-11563.6068
1609.6500	0.1301	0.8699	-11588.9001

1608.6500	0.1281	0.8719	-11613.6279
1607.6500	0.1262	0.8738	-11637.8043
1606.6500	0.1243	0.8757	-11661.4434
1605.6500	0.1225	0.8775	-11684.5587
1604.6500	0.1207	0.8793	-11707.1634
1603.6500	0.1189	0.8811	-11729.2705
1602.6500	0.1172	0.8828	-11750.8924
1601.6500	0.1155	0.8845	-11772.0416
1600.6500	0.1139	0.8861	-11792.7299
1599.6500	0.1123	0.8877	-11812.9689
1598.6500	0.1107	0.8893	-11832.7701
1597.6500	0.1092	0.8908	-11852.1444
1596.6500	0.1077	0.8923	-11871.1027
1595.6500	0.1062	0.8938	-11889.6555
1594.6500	0.1048	0.8952	-11907.8129
1593.6500	0.1034	0.8966	-11925.5850
1592.6500	0.1020	0.8980	-11942.9815
1591.6500	0.1006	0.8994	-11960.0118
1590.6500	0.0993	0.9007	-11976.6851
1589.6500	0.0980	0.9020	-11993.0105
1588.6500	0.0968	0.9032	-12008.9966
1587.6500	0.0955	0.9045	-12024.6519
1586.6500	0.0943	0.9057	-12039.9849
1585.6500	0.0931	0.9069	-12055.0034
1584.6500	0.0920	0.9080	-12069.7155
1583.6500	0.0908	0.9092	-12084.1287
1582.6500	0.0897	0.9103	-12098.2506
1581.6500	0.0886	0.9114	-12112.0883
1580.6500	0.0876	0.9124	-12125.6490
1579.6500	0.0865	0.9135	-12138.9395
1578.6500	0.0855	0.9145	-12151.9666
1577.6500	0.0845	0.9155	-12164.7367
1576.6500	0.0835	0.9165	-12177.2563
1575.6500	0.0826	0.9174	-12189.5315
1574.6500	0.0816	0.9184	-12201.5684
1573.6500	0.0807	0.9193	-12213.3728
1572.6500	0.0798	0.9202	-12224.9505
1571.6500	0.0789	0.9211	-12236.3070
1570.6500	0.0781	0.9219	-12247.4477
1569.6500	0.0772	0.9228	-12258.3780
1568.6500	0.0764	0.9236	-12269.1029
1567.6500	0.0756	0.9244	-12279.6275
1566.6500	0.0748	0.9252	-12289.9567
1565.6500	0.0740	0.9260	-12300.0951
1564.6500	0.0732	0.9268	-12310.0475
1563.6500	0.0725	0.9275	-12319.8183
1562.6500	0.0717	0.9283	-12329.4119
1561.6500	0.0710	0.9290	-12338.8325
1560.6500	0.0703	0.9297	-12348.0845
1559.6500	0.0696	0.9304	-12357.1717
1558.6500	0.0689	0.9311	-12366.0981
1557.6500	0.0682	0.9318	-12374.8676
1556.6500	0.0676	0.9324	-12383.4840
1556.1500	0.0671	0.9329	-12388.6931
1555.9000	0.0669	0.9331	-12391.6446

Phase Region from 1555.84 for:

LIQUID

FCC_A1#1

M7C3

1555.8375	0.0650	0.9350	-12416.4181
1555.7750	0.0622	0.9378	-12453.5554
1555.7125	0.0589	0.9411	-12497.3432
1555.6500	0.0552	0.9448	-12545.5403
1555.5875	0.0513	0.9487	-12596.3233
1555.5250	0.0473	0.9527	-12648.2473
1555.4625	0.0433	0.9567	-12700.1866
1555.4000	0.0393	0.9607	-12751.2745
1555.3375	0.0355	0.9645	-12800.8491
1555.2750	0.0318	0.9682	-12848.4091
1555.2125	0.0283	0.9717	-12893.5793
1555.1500	0.0250	0.9750	-12936.0845
1555.0875	0.0220	0.9780	-12975.7304
1555.0250	0.0191	0.9809	-13012.3915

```
      1554.9625          0.0165          0.9835     -13045.9965
      1554.9000          0.0141          0.9859     -13076.5264
      1554.8375          0.0120          0.9880     -13104.0071
      1554.7750          0.0101          0.9899     -13128.5059
      1554.7125          0.0084          0.9916     -13150.1271
 *** Buffer saved on file tcex48a.POLY3
   ... the command in full is REINITIATE_PLOT_SETTINGS

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is SET_AUTOMATIC_DIAGRAM_A

 Setting automatic diagram axis

   ... the command in full is APPEND_EXPERIMENTAL_DATA
Hard copy of the diagram? /N/:  N
Save coordinates of curve on text file? /N/:  y
File name /scheil/:  tcex48a
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
   ... the command in full is APPEND_EXPERIMENTAL_DATA
   ... the command in full is SET_LABEL_CURVE_OPTION
Any more diagrams? /Y/:  Y
  ..........................................................

        The following axis variables are available

            T --- Temperature in Celsius
         NL/BL --- Mole/mass fraction of liquid
         NS/BS --- Mole/mass fraction of all solid phases
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
      W(ph,el) --- Weight fraction of an element in a phase
      X(ph,el) --- Mole fraction of an element in a phase
      Y(ph,el) --- Site fraction of an element in a phase
     NN(ph,el) --- Distribution of an element in a phases
         NH/BH --- Heat release and Latent heat per mole/gram
        CP/BCP --- Apparent heat capacity per mole/gram

  "el" and "ph" are name of element and phase, respectively
     "*" can be used as a wild character for "el" and "ph"

  ..........................................................

X-axis Variable: ns(fcc)
Y-axis Variable: w(fcc,cr)
Zoom in? /N/:  N
Hard copy of the diagram? /N/:  N
Save coordinates of curve on text file? /N/:  y
File name: /scheil/:  tcex48b
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
   ... the command in full is APPEND_EXPERIMENTAL_DATA
   ... the command in full is SET_LABEL_CURVE_OPTION
Any more diagrams? /Y/:  N
   ... the command in full is ADVANCED_OPTIONS
SYS: @@
SYS: @@ Ignore back diffusion of C in solids and do Scheil with the same alloy
SYS: @@ by choosing option 3 from the Scheil simulation option list.
SYS: @@ also plot solidification and microsegregation diagrams
SYS: @@ save them to files
SYS: @@
SYS: @?<Hit_return_to_continue>
SYS: go sc
   ... the command in full is GOTO_MODULE

         SCHEIL_GULLIVER SIMULATION MODULE VERSION 4.0

 ..........................................................
 .                                                        .
 .       1. Start new simulation                          .
 .       2. Open old file and plot diagram                .
 .       3. Open old file and make another simulation     .
 .                                                        .
 ..........................................................
```

```
Select option /3/:  3
File name /tcex48a.POLY3/:  tcex48a.POLY3
Mass (weight) percent of C /1/:  1
Mass (weight) percent of CR /10/:  10
Temperature (C) /1441/:  1700
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
     Calculated liquidus temperature is 1441.00(C)
     Please enter simulation conditions !

Temperature step (C) /1/:  1
Default stop point? /Y/:  Y
Fast diffusing components: /NONE/:  NONE
Buffer-saving file name /tcex48a.POLY3/:  tcex48b
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
   ... the command in full is ADVANCED_OPTIONS
   ... the command in full is STEP_WITH_OPTIONS

 Phase Region from    1714.15     for:
     LIQUID
 Calculated     4 equilibria

 Phase Region from    1713.15     for:
     LIQUID
     FCC_A1#2
 Calculated   111 equilibria

 Phase Region from    1605.28     for:
     FCC_A1#2
 *** Buffer saved on file: tcex48b.POLY3

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is ENTER_SYMBOL
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 An EXP file tcex48b_EQ.EXP
 has been created to store the equilibrium            solidification results.
   ... the command in full is READ_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

   ... the command in full is ADD_INITIAL_EQUILIBRIUM

 Phase Region from    1714.15     for:
     LIQUID
 Calculated     4 equilibria

 Phase Region from    1713.15     for:
     LIQUID
     FCC_A1#2
 Calculated   176 equilibria

 Phase Region from    1540.21     for:
     LIQUID
     FCC_A1#2
     M7C3
 Calculated    67 equilibria
 *** Buffer saved on file: tcex48b.POLY3
   ... the command in full is REINITIATE_PLOT_SETTINGS

  POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

   ... the command in full is SET_AUTOMATIC_DIAGRAM_A

 Setting automatic diagram axis
```

```
   ... the command in full is APPEND_EXPERIMENTAL_DATA
Hard copy of the diagram? /N/: N
Save coordinates of curve on text file? /N/: y
File name /scheil/: tcex48c
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
   ... the command in full is APPEND_EXPERIMENTAL_DATA
   ... the command in full is SET_LABEL_CURVE_OPTION
Any more diagrams? /Y/: Y
  ......................................................

       The following axis variables are available

            T --- Temperature in Celsius
         NL/BL --- Mole/mass fraction of liquid
         NS/BS --- Mole/mass fraction of all solid phases
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
     W(ph,el) --- Weight fraction of an element in a phase
     X(ph,el) --- Mole fraction of an element in a phase
     Y(ph,el) --- Site fraction of an element in a phase
    NN(ph,el) --- Distribution of an element in a phases
        NH/BH --- Heat release and Latent heat per mole/gram
       CP/BCP --- Apparent heat capacity per mole/gram

  "el" and "ph" are name of element and phase, respectively
     "*" can be used as a wild character for "el" and "ph"

  ......................................................

X-axis Variable: ns(fcc_a1)
Y-axis Variable: w(fcc_a1,cr)
Zoom in? /N/: N
Hard copy of the diagram? /N/: N
Save coordinates of curve on text file? /N/: y
File name: /scheil/: tcex48d
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
   ... the command in full is APPEND_EXPERIMENTAL_DATA
   ... the command in full is SET_LABEL_CURVE_OPTION
Any more diagrams? /Y/: n
   ... the command in full is ADVANCED_OPTIONS
SYS:
SYS: @?<Hit_return_to_continue>
SYS: @@ calculate simple equilibrium solidification of the same alloy
SYS: @@ and compare the results with those of Scheil and ScheiC
SYS: go p-3
   ... the command in full is GOTO_MODULE
POLY_3: read tcex48b
   ... the command in full is READ_WORKSPACES
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 T=1714.15, W(CR)=WCR, W(C)=WC, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: PTERN

 Conditions:
 T=1714.15, W(CR)=WCR, W(C)=WC, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1714.15 K (  1441.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.34983E+01
 Total Gibbs energy -1.01561E+05,  Enthalpy  6.61733E+04,  Volume  7.88681E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.4541E-02  1.0000E-02 3.1364E-03 -8.2160E+04 SER
 CR                      1.0289E-01  1.0000E-01 2.9156E-04 -1.1602E+05 SER
 FE                      8.5257E-01  8.9000E-01 8.4630E-04 -1.0083E+05 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3498E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  8.90000E-01  CR  1.00000E-01  C   1.00000E-02
POLY_3: rei
```

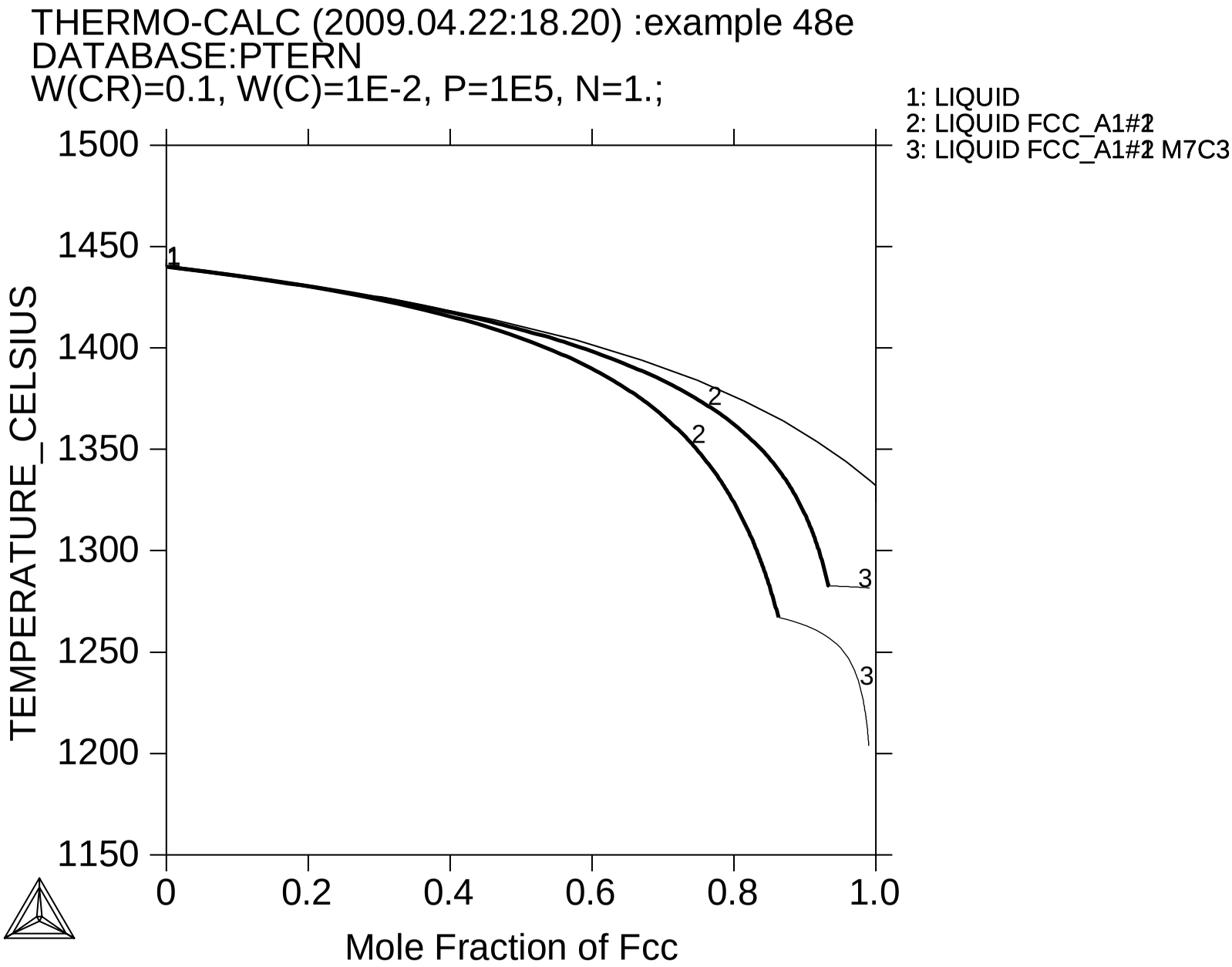
```
   ... the command in full is REINITIATE_MODULE
POLY_3: s-c t=1717.15 w(cr)=0.1 w(c)=0.01 p=1e5 n=1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         7985  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 t 500 1717.15 10
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/:  break-condition
Break condition:  np(liq)=0
POLY_3: sa tcex48c y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  NORMAL
 No initial equilibrium, using default
 Step will start from axis value    1717.15
 Global calculation of initial equilibrium ....OK

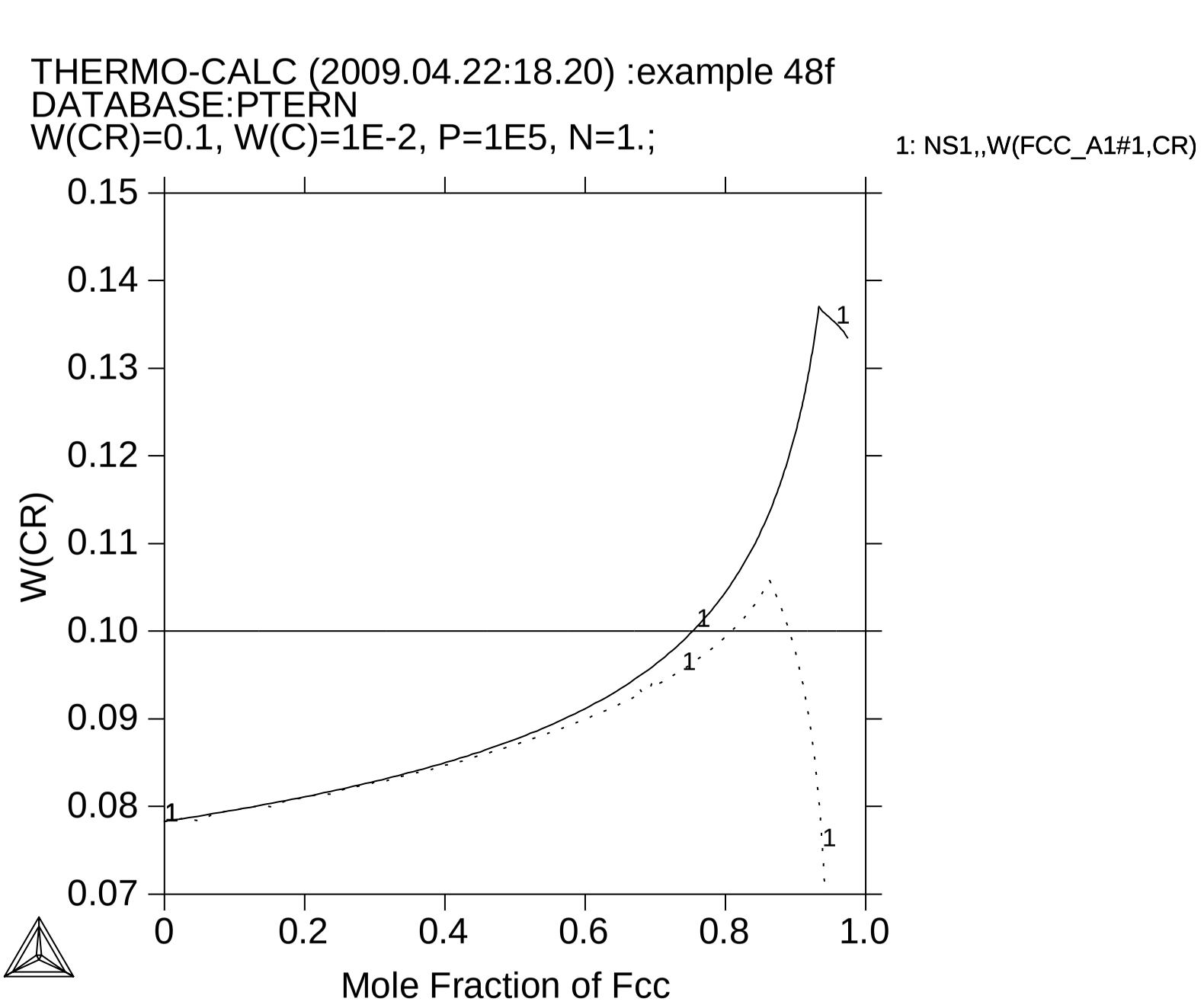
 Phase Region from    1717.15     for:
     LIQUID
 Global check of adding phase at  1.71315E+03
 Calculated     3 equilibria

 Phase Region from    1713.15     for:
     LIQUID
     FCC_A1#2
 Global test at  1.63715E+03 .... OK
 Global check of removing phase at  1.60528E+03
 Calculated    14 equilibria

 Phase Region from    1605.28     for:
     FCC_A1#2
 Calculated     4 equilibria
 *** Buffer saved on file: tcex48c.POLY3
POLY_3: po
   ... the command in full is POST
POST: @@ define a function to get amount of solids
POST: ent fun fs=1-np(liq);
   ... the command in full is ENTER_SYMBOL
POST: @@ plot solidification diagram
POST: s-d-a x fs
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: ap-e y tcex48a.exp tcex48c.exp 0; 1; 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: s-a-te x n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Mole Fraction of Fcc
POST: s-s y n 1160 1460
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 48e
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST:
POST: @@ plot microsegregation which represent the composition profile
POST: @@ of the solid. For equilibrium solidification
POST: @@ there is no solute segregation and the composition of
POST: @@ solidified solid is uniform.
POST: s-d-a x fs
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(cr)
   ... the command in full is SET_DIAGRAM_AXIS
POST: ap-e y tcex48b.exp tcex48d.exp 0; 1; 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
```

POST: **s-a-te x n**
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : **Mole Fraction of Fcc**
POST: **s-s y n 0.075 0.15**
... the command in full is SET_SCALING_STATUS
POST: **set-title example 48f**
POST: **pl**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **set-inter**
... the command in full is SET_INTERACTIVE_MODE
POST: CPU time 6 seconds


THERMO-CALC (2009.04.22:18.20) :example 48e
DATABASE:PTERN
W(CR)=0.1, W(C)=1E-2, P=1E5, N=1.;
1: LIQUID
2: LIQUID FCC_A1#2
3: LIQUID FCC_A1#2 M7C3
TEMPERATURE_CELSIUS
1500
1450
1400
1350
1300
1250
1200
1150
0
0.2
0.4
0.6
0.8
1.0
Mole Fraction of Fcc


THERMO-CALC (2009.04.22:18.20) :example 48f
DATABASE:PTERN
W(CR)=0.1, W(C)=1E-2, P=1E5, N=1.;
1: NS1,,W(FCC_A1#1,CR)
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
W(CR)
0
0.2
0.4
0.6
0.8
1.0
Mole Fraction of Fcc
1
1
1
1
1

49

Quasichemical Model via G-E-S

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Example showing entering parameter for FACT quasichemical liquid model
SYS: @@ and calculating the sulfur activity
SYS:
SYS: set-log ex49,,,
SYS:
SYS:  go gibbs
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
 First version released 1-Jan-78, last update 20-Nov-2007

GES:  ent-el  /- VA CU S
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
GES:  am_el_d /-  ELECTRON_GAS       0.0000E+00  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES:  am_el_d VA  VACUUM             0.0000E+00  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES:  am_el_d CU  FCC_A1             6.3546E+01  5.0041E+03  3.3150E+01 1
   ... the command in full is AMEND_ELEMENT_DATA
GES:  am_el_d S   FC_ORTHORHOMBIC    3.2066E+01  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES:
GES:
GES: @@ The quasichemical model requires species entered with the
GES: @@ stoichiometry.  The factor 2/ZZ is needed
GES: @@ for the pure elements and 1/ZZ for the compounds.
GES: @@ For Cu ZZ=0.9294 and 2/ZZ_Cu=2.15193
GES: @@ For S  ZZ=1.8366 and 2/ZZ_S=1.08897
GES: @@ For CuS the stoichiometries are thus 1/ZZ_Cu=1.07596 and
GES: @@ 1/ZZ_S=0.54448
GES:
GES:  enter-specie CUQ                          CU2.15193
   ... the command in full is ENTER_SPECIES
GES:  enter-specie CUQS                         CU1.07596S0.54448
   ... the command in full is ENTER_SPECIES
GES:  enter-specie S2                           S2
   ... the command in full is ENTER_SPECIES
GES:  enter-specie SQ                           S1.08897
   ... the command in full is ENTER_SPECIES
GES:
GES:
GES: @@ The Gibbs energy difference between FCC-Cu and quasichemical liquid-Cu
GES:
GES:  ent-sym fun GQCU  2.98150E+02  +16547-7.6815*T;   6.00000E+03   N
   ... the command in full is ENTER_SYMBOL
GES:
GES:
GES: @@ The Gibbs energy difference between GAS-S and quasichemical liquid-S
GES:
GES:  ent-sym fun GQS   2.98150E+02  -65357+165.396*T-13.513*T*LN(T);
   ... the command in full is ENTER_SYMBOL
HIGH TEMPERATURE LIMIT /6000/:       6.00000E+03   N
GES:
GES:
GES:
GES: @@ Gibbs energies for the pure elements and gases refered to SER
GES:  ent-sym fun GHSERCU   2.98150E+02  -7770.458+130.485403*T
   ... the command in full is ENTER_SYMBOL
&       -24.112392*T*LN(T)-.00265684*T**2+1.29223E
```

```
&       -07*T**3+52478*T**(-1);  1.35802E+03  Y
FUNCTION:       -13542.33+183.804197*T-31.38*T*LN(T)+3.64643E+29*T**(-9);
HIGH TEMPERATURE LIMIT /6000/:         3.20000E+03 N
GES:  ent-sym fun GS2GAS    2.98150E+02  +117374.548+2.98629558*T
   ... the command in full is ENTER_SYMBOL
&       -34.09678*T*LN(T)-.002325464*T**2+1.85480167E-07*T**3
&       +128593.6*T**(-1);  1.00000E+03  Y
FUNCTION:       +117352.438+2.50383258*T-34.04744*T*LN(T)-.0021150245*T**2
&       +9.16602333E-08*T**3+175718.45*T**(-1);  3.40000E+03  Y
FUNCTION:       +124361.091+14.5182895*T-36.1923*T*LN(T)-5.930925E-04*T**2
&       -7.54259333E-09*T**3-7484105*T**(-1);  6.00000E+03  N
GES:  ent-sym fun GSSLIQ    2.98150E+02  -4001.549+77.889686*T
   ... the command in full is ENTER_SYMBOL
&       -15.504*T*LN(T)-.018629*T**2-2.4942E-07*T**3
&       -113945*T**(-1);  3.88360E+02  Y
FUNCTION:       -5285183.35+118449.585*T-19762.4*T*LN(T)+32.79275*T**2
&       -.0102214167*T**3+2.646735E+08*T**(-1);  4.28150E+02  Y
FUNCTION:       -8174995.23+319914.078*T-57607.3*T*LN(T)+135.3045*T**2
&       -.0529973333*T**3;  4.32250E+02  Y
FUNCTION:       -219408.801+7758.83993*T-1371.85*T*LN(T)+2.845035*T**2
&       -.00101380333*T**3;  4.53150E+02  Y
FUNCTION:       +92539.872-1336.36627*T+202.958*T*LN(T)-.2531915*T**2
&       +5.18835E-05*T**3-8202200*T**(-1);  7.17000E+02  Y
FUNCTION:        -6889.972+176.35482*T-32*T*LN(T);  1.30000E+03  N
GES:  ent-sym fun GCULIQ    2.98150E+02  +12964.84-9.510243*T
   ... the command in full is ENTER_SYMBOL
&       -5.83932E-21*T**7+GHSERCU ;  1.35802E+03  Y
FUNCTION:       +13495.4-9.920463*T-3.64643E+29*T**(-9)+GHSERCU ;
HIGH TEMPERATURE LIMIT /6000/:         3.20000E+03  N
GES:
GES:
GES:
GES:  ent-phase GAS  G,  1   S2 ;  N N
   ... the command in full is ENTER_PHASE
GES:
GES:
GES:  ent-param G(GAS,S2;0)  2.98150E+02  +GS2GAS +RTLNP ;
   ... the command in full is ENTER_PARAMETER
 G(GAS,S2;0)- 2 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/:           6.00000E+03   N
GES:
GES:
GES:
GES:  ent-phase FCC_A1  ,  1   CU ;  N N
   ... the command in full is ENTER_PHASE
GES:  amend_phase FCC_A1 magnetic  -3.0    2.80000E-01
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES:
GES:  ent-param G(FCC_A1,CU;0) 2.98150E+02 +GHSERCU; 3.20000E+03  N
   ... the command in full is ENTER_PARAMETER
 G(FCC_A1,CU;0)-G(FCC_A1,CU;0)
GES:
GES:
GES:
GES:  ent-phase QUASI  L,  1    CUQ,CUQS,SQ ;  N N
   ... the command in full is ENTER_PHASE
GES:
GES:
GES: @@ The stoichiometry parameter for pure Cu is 2/ZZ,
GES: @@ the stoichiometry ratio
GES:
GES:  ent-param VK(QUASI,CUQ;0)  2.98150E+02 .9294; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 VK(QUASI,CUQ;0)
GES:
GES: @@ The energy parameter for pure Cu (factor is 2/VK)
GES:
GES:  ent-param G(QUASI,CUQ;0)  2.98150E+02  +2.15193*GCULIQ
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ;0)-2.15193 G(FCC_A1,CU;0)
&        +2.15193*GQCU ;   6.00000E+03   N
GES:
GES: @@ The Gibbs energy parameter for the molecule CUQS
```

```
GES: @@ (factors 1/ZZ_cu and 1/ZZ_s)
GES:
GES:  ent-param G(QUASI,CUQS;0)  2.98150E+02  +1.07596*GCULIQ
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQS;0)-1.07596 G(FCC_A1,CU;0)-0.54448 G(FC_ORTHORHOMBIC,S;0)
&        +1.075963*GQCU+.54448*GSSLIQ ;  6.00000E+03   N
GES:
GES:
GES: @@ The stoichiometry parameter for pure S is 2/ZZ
GES:
GES:  ent-param VK(QUASI,SQ;0) 2.98150E+02 1.8366; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 VK(QUASI,SQ;0)
GES:
GES: @@ The energy parameter for pure S (factor is 2/VK)
GES:
GES:  ent-param G(QUASI,SQ;0)  2.98150E+02  +1.08897*GSSLIQ ;
   ... the command in full is ENTER_PARAMETER
 G(QUASI,SQ;0)-1.08897 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/:           6.00000E+03   N
GES:
GES: @@ The mixing terms
GES:
GES:  ent-param G(QUASI,CUQ,CUQS;0) 2.98150E+02  -82768; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;0)
GES:  ent-param G(QUASI,CUQ,CUQS;1) 2.98150E+02  -32070; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;1)
GES:  ent-param G(QUASI,CUQ,CUQS;2) 2.98150E+02  68734; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;2)
GES:  ent-param G(QUASI,CUQ,CUQS;3) 2.98150E+02  -84194+50*T;
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;3)
HIGH TEMPERATURE LIMIT /6000/:      6.00000E+03   N
GES:  ent-param G(QUASI,CUQ,CUQS;4) 2.98150E+02  -43638; 6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;4)
GES:  ent-param G(QUASI,CUQ,CUQS;5) 2.98150E+02  +20*T;  6.00000E+03   N
   ... the command in full is ENTER_PARAMETER
 G(QUASI,CUQ,CUQS;5)
GES:
GES:
GES: @@ This command makes the entropy calculation according to
GES: @@ FACT quasichemical model
GES:
GES: amend-phase-description QUASI quasi-fact00
GES:
GES: @@ Binary excess Legendre with 1 as independent
GES: @@ Note that the order of the species are important!
GES:
GES: amend-phase-description QUASI excess
MODEL NAME /REDLICH-KISTER_MUGGIANU/:  mixed
First (the independent) constituent: CUQ
Second (the dependent) constituent: CUQS
Excess model type: /LEGENDRE/:  Legendre
 Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent: NONE
GES:
GES:
GES:
GES: list-data
OUTPUT FILE: /SCREEN/:
OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH          DATE 2009- 4-22
 FROM DATABASE: User data 2009. 4.22

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS             0.0000E+00  0.0000E+00  0.0000E+00
```

```
 0 VA   VACUUM                   0.0000E+00  0.0000E+00  0.0000E+00
 1 CU   FCC_A1                   6.3546E+01  5.0041E+03  3.3150E+01
 2 S    FC_ORTHORHOMBIC          3.2066E+01  0.0000E+00  0.0000E+00

SPECIES                                  STOICHIOMETRY
  1 CU                                   CU
  2 CUQ                                  CU2.15193
  3 CUQS                                 CU1.07596S0.54448
  4 S                                    S
  5 S2                                   S2
  6 SQ                                   S1.08897
  7 VA                                   VA

GAS
   CONSTITUENTS: S2

     G(GAS,S2;0)- 2 G(FC_ORTHORHOMBIC,S;0) = +GS2GAS+RTLNP

QUASI
$ QUASICHEMICAL-FACT00 ENTROPY CONTRIBUTION
   CONSTITUENTS: CUQ,CUQS,SQ

     VK(QUASI,CUQ;0) = .9294
     G(QUASI,CUQ;0)-2.15193 G(FCC_A1,CU;0) = +2.15193*GCULIQ+2.15193*GQCU
     G(QUASI,CUQS;0)-1.07596 G(FCC_A1,CU;0)-0.54448 G(FC_ORTHORHOMBIC,S;0) =
           +1.07596*GCULIQ+1.075963*GQCU+.54448*GSSLIQ
     VK(QUASI,SQ;0) = 1.8366
     G(QUASI,SQ;0)-1.08897 G(FC_ORTHORHOMBIC,S;0) = +1.08897*GSSLIQ
$ Binary excess model Legendre with CUQ as independent
     L(QUASI,CUQ,CUQS;0) = -82768
     L(QUASI,CUQ,CUQS;1) = -32070
     L(QUASI,CUQ,CUQS;2) = 68734
     L(QUASI,CUQ,CUQS;3) = -84194+50*T
     L(QUASI,CUQ,CUQS;4) = -43638
     L(QUASI,CUQ,CUQS;5) = +20*T

FCC_A1
ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
     Magnetic function below Curie Temperature
     +1-.860338755*TAO**(-1)-.17449124*TAO**3-.00775516624*TAO**9
     -.0017449124*TAO**15
     Magnetic function above Curie Temperature
      -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)
     -2.84601512E-04*TAO**(-25)
   CONSTITUENTS: CU

     G(FCC_A1,CU;0)-G(FCC_A1,CU;0) =    298.15<T< 3200.00: +GHSERCU

SYMBOL        STATUS   VALUE/FUNCTION
  1 R         80000000  8.3145100E+00
  2 RTLNP     20000000 +R*T*LN(1E-05*P)
103 GQCU      20000000 +16547-7.6815*T
104 GQS       20000000 -65357+165.396*T-13.513*T*LN(T)
105 GHSERCU   20000000
      298.15<T< 1358.02: -7770.458+130.485403*T-24.112392*T*LN(T)
    -.00265684*T**2+1.29223E-07*T**3+52478*T**(-1)
     1358.02<T< 3200.00: -13542.33+183.804197*T-31.38*T*LN(T)
    +3.64643E+29*T**(-9)
106 GS2GAS    20000000
      298.15<T< 1000.00: +117374.548+2.98629558*T-34.09678*T*LN(T)
    -.002325464*T**2+1.85480167E-07*T**3+128593.6*T**(-1)
     1000.00<T< 3400.00: +117352.438+2.50383258*T-34.04744*T*LN(T)
    -.0021150245*T**2+9.16602333E-08*T**3+175718.45*T**(-1)
     3400.00<T< 6000.00: +124361.091+14.5182895*T-36.1923*T*LN(T)
    -5.930925E-04*T**2-7.54259333E-09*T**3-7484105*T**(-1)
107 GSSLIQ    20000000
      298.15<T<  388.36: -4001.549+77.889686*T-15.504*T*LN(T)-.018629*T**2
    -2.4942E-07*T**3-113945*T**(-1)
      388.36<T<  428.15: -5285183.35+118449.585*T-19762.4*T*LN(T)
    +32.79275*T**2-.0102214167*T**3+2.646735E+08*T**(-1)
      428.15<T<  432.25: -8174995.23+319914.078*T-57607.3*T*LN(T)
    +135.3045*T**2-.0529973333*T**3
      432.25<T<  453.15: -219408.801+7758.83993*T-1371.85*T*LN(T)
    +2.845035*T**2-.00101380333*T**3
```

```
       453.15<T<  717.00: +92539.872-1336.36627*T+202.958*T*LN(T)
     -.2531915*T**2+5.18835E-05*T**3-8202200*T**(-1)
       717.00<T< 1300.00: -6889.972+176.35482*T-32*T*LN(T)
 108 GCULIQ    20000000
       298.15<T< 1358.02: +12964.84-9.510243*T-5.83932E-21*T**7+GHSERCU
      1358.02<T< 3200.00: +13495.4-9.920463*T-3.64643E+29*T**(-9)+GHSERCU

GES:
GES: @?<Hit_return_to_continue>
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3:
POLY_3:
POLY_3:
POLY_3: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 FCC_A1                 ENTERED    0.00000000E+00  0.00000000E+00
 QUASI                  ENTERED    0.00000000E+00  0.00000000E+00
 GAS                    ENTERED    0.00000000E+00  0.00000000E+00
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p q gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:  ENTERED
Start value, number of moles /0/:  0
POLY_3:
POLY_3:
POLY_3: s-c t=1473 p=1e5 n=1 x(s)=.33
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1978  grid points in            1  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     1  s
POLY_3: l-e
   ... the command in full is LIST_EQUILIBRIUM
Output file: /SCREEN/:
Options /VWCS/:  VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=1473, P=1E5, N=1, X(S)=0.33
 DEGREES OF FREEDOM 0

 Temperature   1473.00 K (  1199.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.31576E+01
 Total Gibbs energy -1.24169E+05,  Enthalpy  1.52783E+04,  Volume  0.00000E+00

 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 CU                     6.7000E-01  8.0094E-01 8.2231E-04 -8.6997E+04 SER
 S                      3.3000E-01  1.9906E-01 8.3318E-08 -1.9964E+05 SER

 QUASI                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3158E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  8.00936E-01  S   1.99064E-01
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-r-s s gas
   ... the command in full is SET_REFERENCE_STATE
Temperature /*/:  *
Pressure /1E5/:  1E5
POLY_3: sh acr(s)
   ... the command in full is SHOW_VALUE
 ACR(S)=2.1652884E-3
POLY_3: @?<Hit_return_to_continue>
POLY_3: s-a-v 1 x(s)
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/:  .3
Max value /1/:  .4
Increment /.0025/:  .0025
```

```
POLY_3: save tcex49 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:  NORMAL
 No initial equilibrium, using default
 Step will start from axis value   0.330000
 Global calculation of initial equilibrium ....OK

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.61133E-01
 Calculated    15 equilibria

 Phase Region from   0.361133     for:
     GAS
     QUASI
 Global test at  3.80000E-01 .... OK
 Terminating at   0.400000
 Calculated    19 equilibria

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.10000E-01 .. Creating a new composition set QUASI#2
 Backtracking to find phase change for QUASI#2
 Global test at  3.27500E-01 .... OK
 Global test at  3.22500E-01 .... OK
 Global test at  3.17500E-01 .... OK
 Global test at  3.12500E-01 .... OK
 Global check of adding phase at  3.11581E-01
 Calculated    11 equilibria

 Phase Region from   0.311581     for:
     QUASI#1
     QUASI#2
 Terminating at   0.300000
 Calculated     8 equilibria
 *** Buffer saved on file: tcex49.POLY3
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y acr(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49a
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: set-title example 49b
POST: pl
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: s-d-a y y(quasi,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: s-a-ty y lin
   ... the command in full is SET_AXIS_TYPE
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 49c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
```

```
POST:
POST:
POST:@?
POST: back
POLY_3: read tcex49
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-c t=1573
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1978  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value   0.330000
 Global calculation of initial equilibrium ....OK

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.56605E-01
 Calculated    13 equilibria

 Phase Region from   0.356605     for:
     GAS
     QUASI
 Global test at  3.75000E-01 .... OK
 Global test at  4.00000E-01 .... OK
 Terminating at   0.400000
 Calculated    21 equilibria

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.10000E-01 .... OK
 Terminating at   0.300000
 Calculated    15 equilibria
 *** Buffer saved on file: tcex49.POLY3
POLY_3:
POLY_3: read tcex49
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-c t=1673
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1978  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value   0.330000
 Global calculation of initial equilibrium ....OK

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.52789E-01
 Calculated    12 equilibria

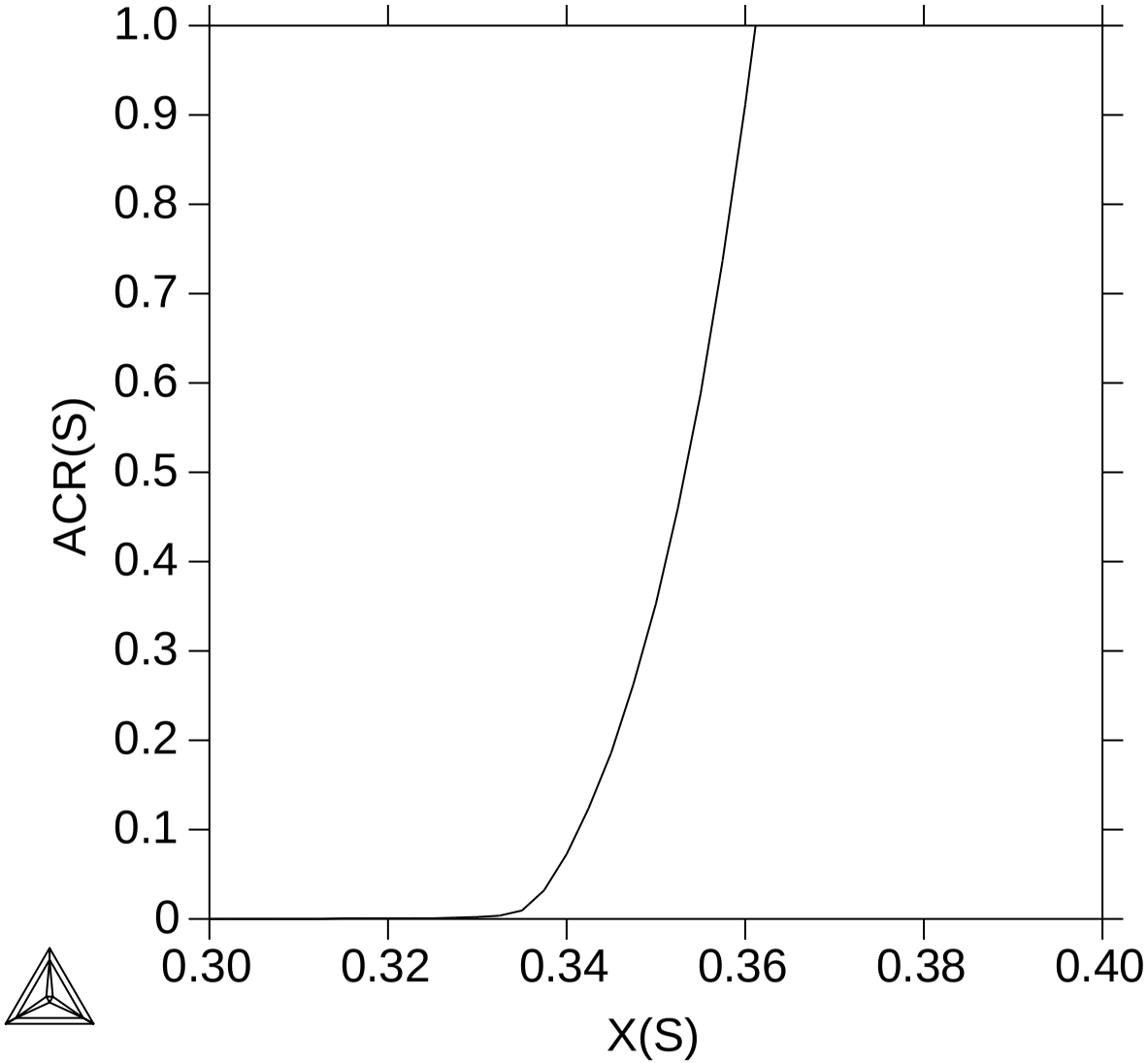
 Phase Region from   0.352789     for:
     GAS
     QUASI
 Global test at  3.72500E-01 .... OK
 Global test at  3.97500E-01 .... OK
```

```
 Terminating at   0.400000
 Calculated    22 equilibria

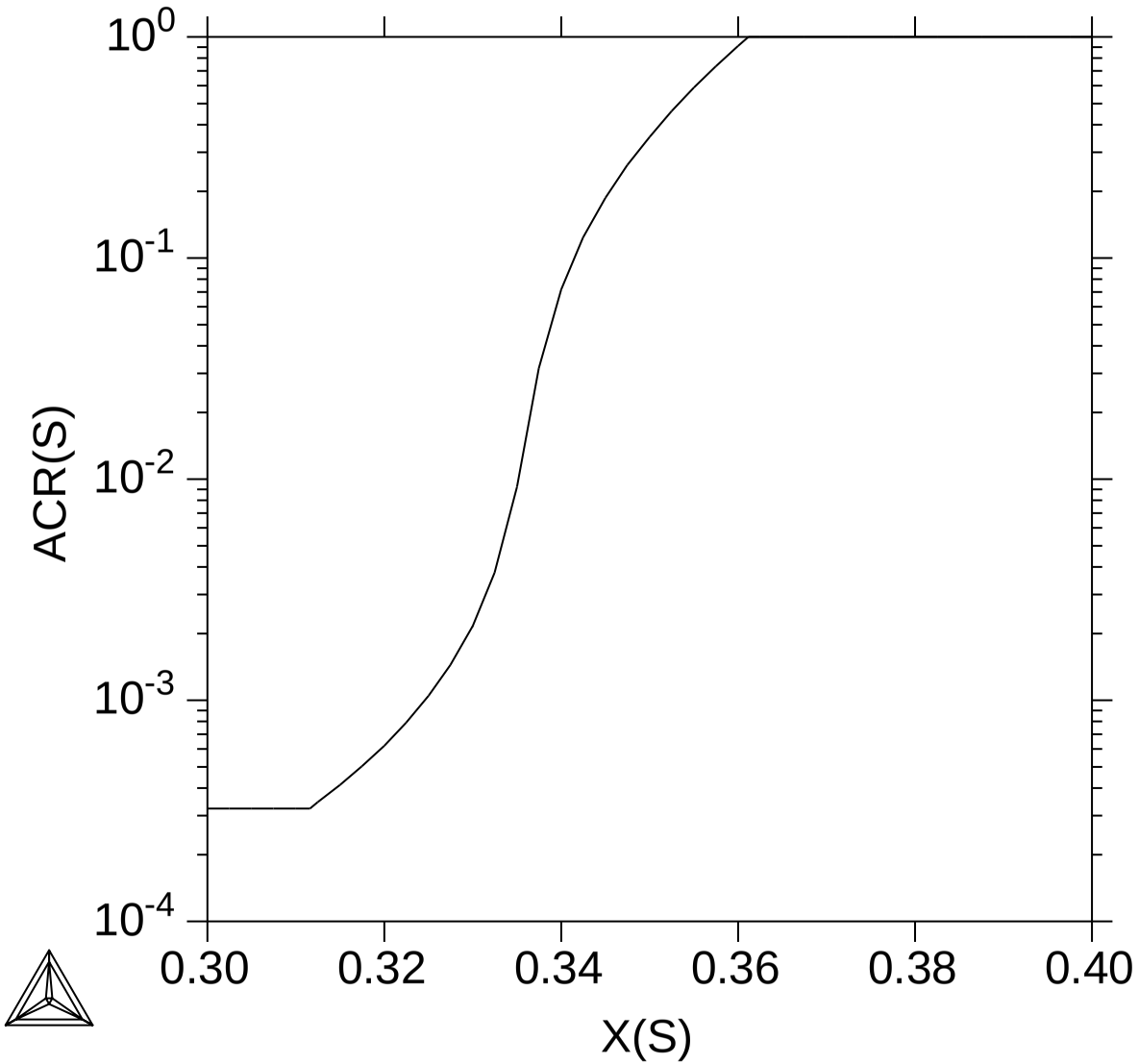
 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.10000E-01 .... OK
 Terminating at   0.300000
 Calculated    15 equilibria
 *** Buffer saved on file: tcex49.POLY3
POLY_3:
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-d-a y mur(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49d
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
 The composition set QUASI#2 created from the store file
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           10  seconds
```

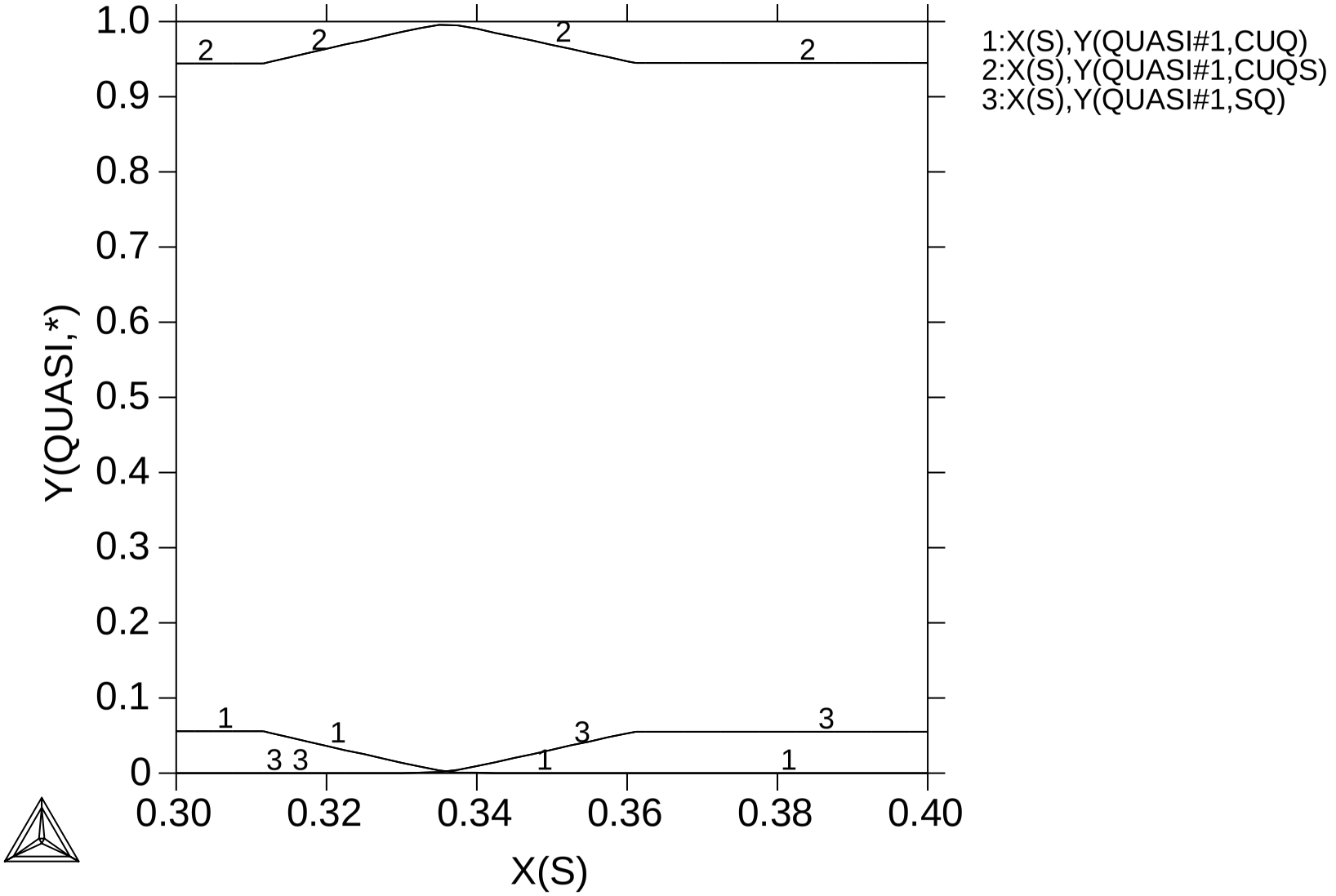
THERMO-CALC (2009.04.22:18.23) :example 49a
DATABASE:User data 2009. 4.22
T=1473, P=1E5, N=1;



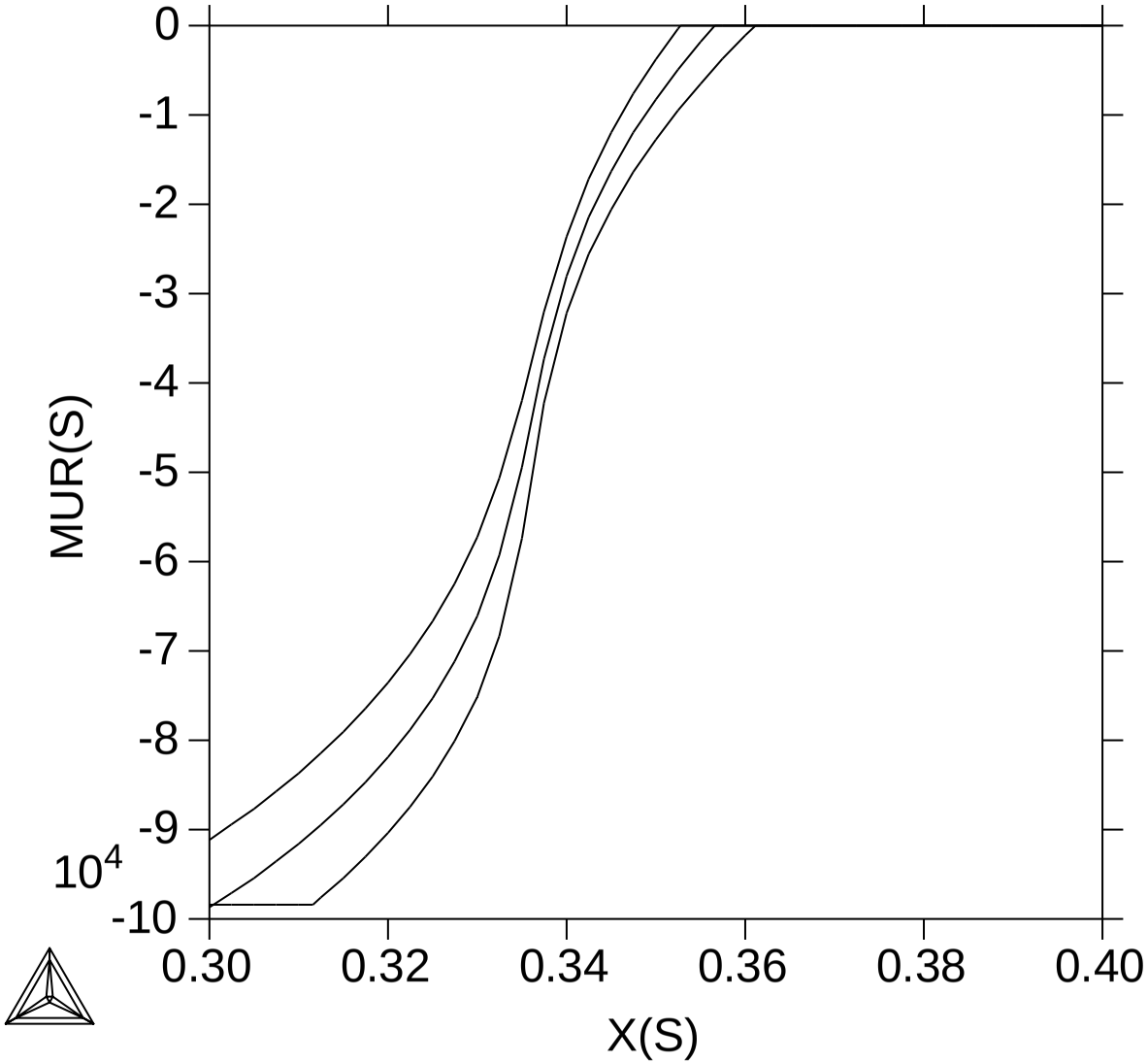
THERMO-CALC (2009.04.22:18.23) :example 49b
DATABASE:User data 2009. 4.22
T=1473, P=1E5, N=1;



THERMO-CALC (2009.04.22:18.23) :example 49c
DATABASE:User data 2009. 4.22
T=1473, P=1E5, N=1;



THERMO-CALC (2009.04.22:18.24) :example 49d
DATABASE:User data 2009. 4.22
T=1673, P=1E5, N=1.;



50

Quasichemical Model via TDB

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ Calculation of Fig 3+4 in Kongoli et al
SYS: @@ Metall. Mater. Trans. B, 29B(1998)591.
SYS: @@ Fe-S
SYS:
SYS: set-log ex50,,,
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw user tcex50
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

TDB_USER: d-sys fe s
   ... the command in full is DEFINE_SYSTEM
 FE                      S  DEFINED
TDB_USER: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE lattice stabilities, Calphad 1991'
  'Kongoli, Dessureault and Pelton, Met Trans B, 29B (1998) p 591-601'
 AFTER ...
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p quasi=ent 1
   ... the command in full is CHANGE_STATUS
POLY_3: s-r-s s quasi * 1E5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: enter fun lng=log(acr(s)/x(s));
   ... the command in full is ENTER_SYMBOL
POLY_3: s-c t=1573 p=1e5 n=1 x(s)=.35
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in           1  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     2  s
POLY_3: s-a-v 1 x(s) 0 .6,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: s-c t=1473
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
```

```
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1573
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1673
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1773
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1873
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: save tcex50 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK

 Phase Region from   0.350000     for:
     QUASI
 Global test at  4.70000E-01 .... OK
 Terminating at   0.600000
 Calculated    20 equilibria

 Phase Region from   0.350000     for:
     QUASI
 Global test at  2.30000E-01 .. Creating a new composition set QUASI#2
 Backtracking to find phase change for QUASI#2
 Global test at  3.35000E-01 .... OK
 Global test at  3.05000E-01 .... OK
 Global test at  2.75000E-01 .... OK
 Global test at  2.57000E-01 .... OK
 Global check of adding phase at  2.55243E-01
 Calculated    11 equilibria

 Phase Region from   0.255243     for:
```

```
    QUASI#1
    QUASI#2
 Global test at  1.46000E-01 .... OK
 Global check of removing phase at  1.39331E-01
 Calculated    11 equilibria

 Phase Region from   0.139331     for:
    QUASI#2
 Global test at  2.60000E-02 .... OK
 Backtracking to find phase change for QUASI#1
 Global test at  1.31000E-01 .... OK
 Global test at  1.01000E-01 .... OK
 Global test at  7.10000E-02 .... OK
 Global test at  4.10000E-02 .... OK
 Global test at  1.10000E-02 .... OK
 Backtracking to find phase change for QUASI#1
 Global check of adding phase at  5.03828E-02
 Calculated    11 equilibria

       :
       :
       :

 Phase Region from   0.350000     for:
    QUASI#1
 Global test at  4.70000E-01 .... OK
 Terminating at   0.600000
 Calculated    20 equilibria

 Phase Region from   0.350000     for:
    QUASI#1
 Global test at  2.30000E-01 .... OK
 Global test at  8.00000E-02 .... OK
 Terminating at   0.123222E-10
 Calculated    27 equilibria

 Phase Region from   0.350000     for:
    QUASI#1
 Global test at  4.70000E-01 .... OK
 Terminating at   0.600000
 Calculated    20 equilibria

 Phase Region from   0.350000     for:
    QUASI#1
 Global test at  2.30000E-01 .... OK
 Global test at  8.00000E-02 .... OK
 Terminating at   0.122058E-10
 Calculated    27 equilibria
 *** Buffer saved on file: tcex50.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y lng
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n -10 -1
   ... the command in full is SET_SCALING_STATUS
POST: set-title log(gamma_S) in Fe-S liquid
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: back
POLY_3: read tcex50
   ... the command in full is READ_WORKSPACES
POLY_3: rei
   ... the command in full is REINITIATE_MODULE
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p quasi=ent 1
   ... the command in full is CHANGE_STATUS
POLY_3: s-r-s s quasi * 1E5
```

```
   ... the command in full is SET_REFERENCE_STATE
POLY_3: enter fun lng=log(acr(s)/x(s));
   ... the command in full is ENTER_SYMBOL
POLY_3: s-c t=1773 p=1e5 n=1 x(s)=.1
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in           1  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     2  s
POLY_3: save tcex50 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: s-a-v 1 x(s) 0 .14 ,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1823
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1873
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in           1  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     2  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1923
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1973
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=2023
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in           0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: step normal
   ... the command in full is STEP_WITH_OPTIONS
```

```
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK
 Global calculation of initial equilibrium ....OK

 Phase Region from   0.100000     for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000     for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.123099E-10
 Calculated    32 equilibria

 Phase Region from   0.100000     for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000     for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.122501E-10
 Calculated    32 equilibria

       :
       :
       :

 Phase Region from   0.100000     for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000     for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.120889E-10
 Calculated    32 equilibria

 Phase Region from   0.100000     for:
     QUASI
 Global test at  1.28000E-01 .... OK
 Terminating at   0.140000
 Calculated    15 equilibria

 Phase Region from   0.100000     for:
     QUASI
 Global test at  7.20000E-02 .... OK
 Global test at  3.70000E-02 .... OK
 Global test at  2.00000E-03 .... OK
 Terminating at   0.120406E-10
 Calculated    32 equilibria
 *** Buffer saved on file: tcex50.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y lng
   ... the command in full is SET_DIAGRAM_AXIS
```

POST: **s-s x n 0 .14**
   ... the command in full is SET_SCALING_STATUS
POST: **s-s y n -6.5 -3.5**
   ... the command in full is SET_SCALING_STATUS
POST: **set-title log(gamma_S)in Fe-S liquid**
POST: **plot**
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: **@?<Hit_return_to_continue>**
POST: **back**
POLY_3: **read tcex50**
   ... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: **rei**
   ... the command in full is REINITIATE_MODULE
POLY_3: **s-c x(s)=.01 t=1900 n=1 p=1e5**
   ... the command in full is SET_CONDITION
POLY_3: **c-e**
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated   1981 grid points in   0 s
 Found the set of lowest grid points in   0 s
 Calculated POLY solution   1 s, total time   1 s
POLY_3: **l-e,,,,,**
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =   1, label A0 , database: USER

 Conditions:
 X(S)=1E-2, T=1900, N=1, P=1E5
 DEGREES OF FREEDOM 0

 Temperature   1900.00 K (1626.85 C), Pressure 1.000000E+05
 Number of moles of components 1.00000E+00, Mass in grams 5.56092E+01
 Total Gibbs energy -1.19028E+05, Enthalpy 7.56841E+04, Volume 0.00000E+00

 Component   Moles   W-Fraction Activity   Potential Ref.stat
 FE   9.9000E-01 9.9423E-01 5.9397E-04 -1.1736E+05 SER
 S   1.0000E-02 5.7663E-03 5.9092E-05 -1.5381E+05 QUASI

 QUASI   Status ENTERED   Driving force 0.0000E+00
 Moles 1.0000E+00, Mass 5.5609E+01, Volume fraction 0.0000E+00 Mass fractions:
 FE 9.94234E-01 S   5.76631E-03
POLY_3: **@?<Hit_return_to_continue>**
POLY_3: **add -2**
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: **s-c t=1200**
   ... the command in full is SET_CONDITION
POLY_3: **c-e**
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated   1981 grid points in   0 s
 Found the set of lowest grid points in   0 s
 Calculated POLY solution   1 s, total time   1 s
POLY_3: **add 1**
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: **s-a-v 1 x(s) 0 .5 0.01**
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: **s-a-v 2 t 1000 2000 10**
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: **save tcex50 y**
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: **map**
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

```
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4

 Phase region boundary   1 at:   5.000E-03  1.792E+03
  ** BCC_A2
     QUASI
 Calculated           18  equilibria

 Phase region boundary   2 at:   5.000E-03  1.792E+03
  ** BCC_A2
     QUASI
 Calculated.           21  equilibria

 Phase region boundary   3 at:   6.305E-02  1.667E+03
  ** BCC_A2
  ** FCC_A1
     QUASI

 Phase region boundary   4 at:   6.305E-02  1.667E+03
  ** FCC_A1
     QUASI
 Calculated.          162  equilibria

       :
       :
       :

 Phase region boundary   8 at:   0.000E+00  1.667E+03
     BCC_A2
  ** FCC_A1

 Phase region boundary   9 at:   6.305E-02  1.667E+03
  ** BCC_A2
     QUASI
 Calculated           65  equilibria

 Phase region boundary  10 at:   2.243E-01  1.200E+03
  ** FCC_A1
     QUASI
 Calculated.            3  equilibria
 Terminating at known equilibrium

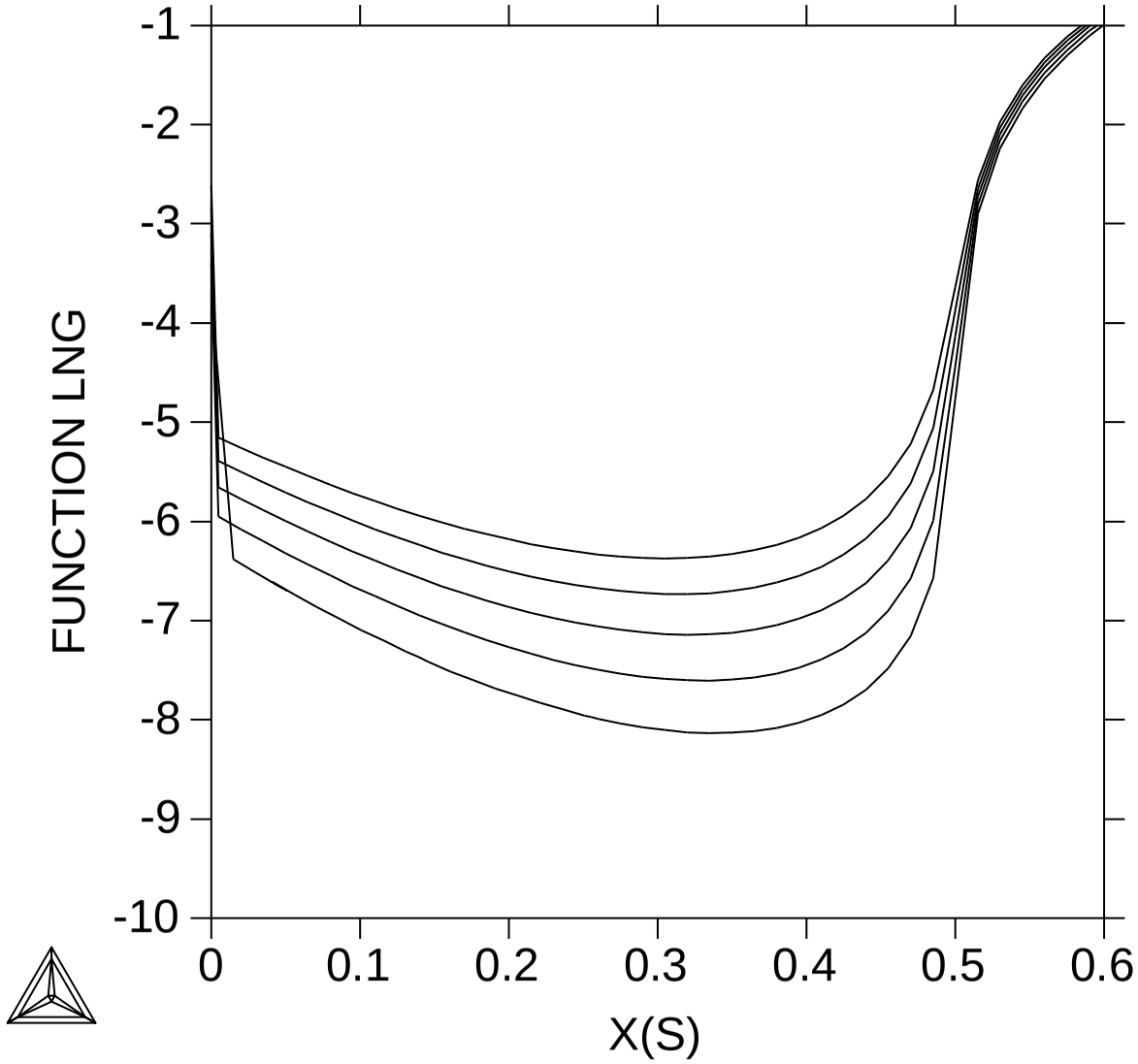
 Phase region boundary  11 at:   2.243E-01  1.200E+03
  ** FCC_A1
     QUASI
 Calculated.          260  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: tcex50.POLY3
 CPU time for mapping          18  seconds
POLY_3: po
   ... the command in full is POST

  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

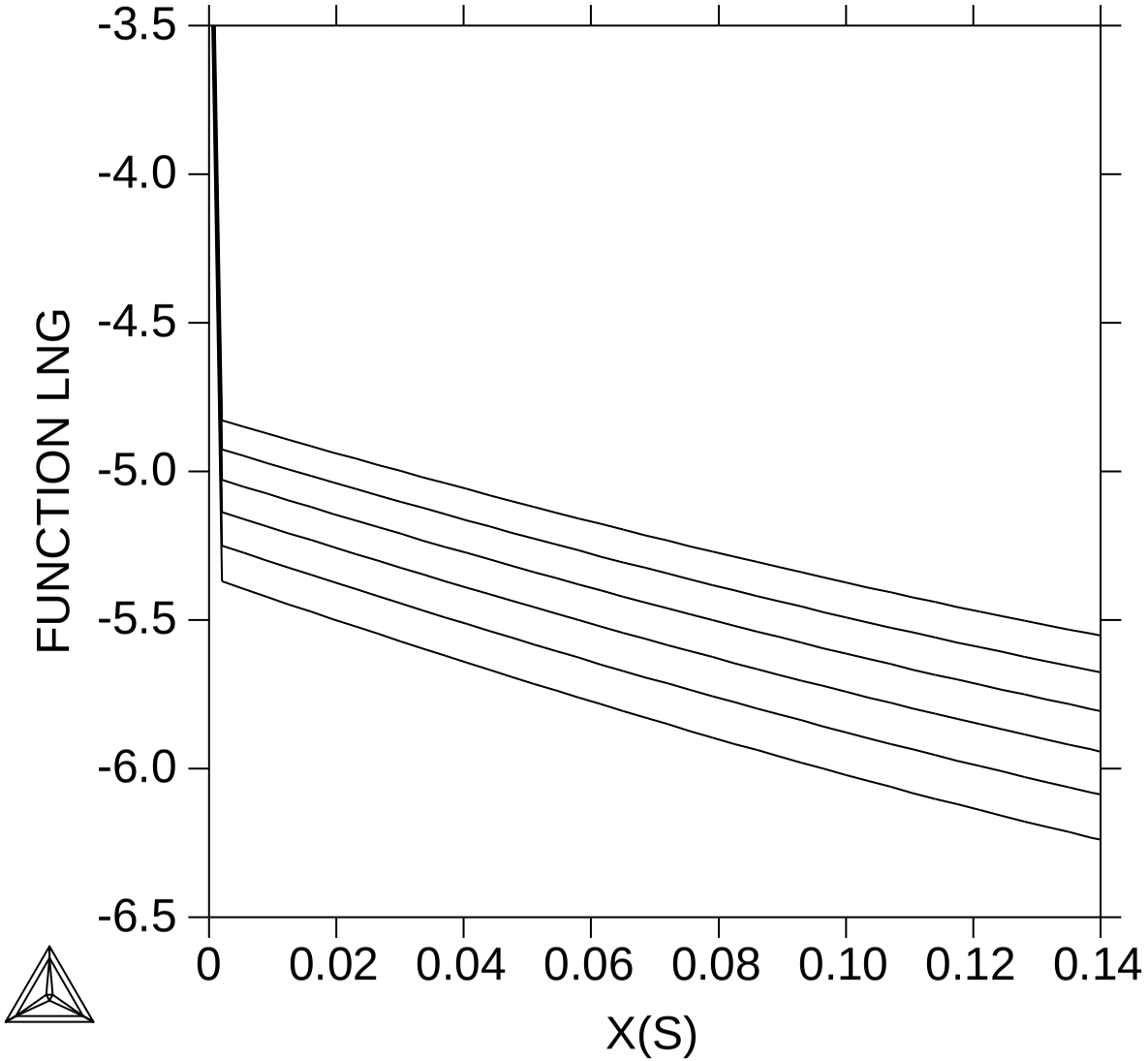
 Setting automatic diagram axis

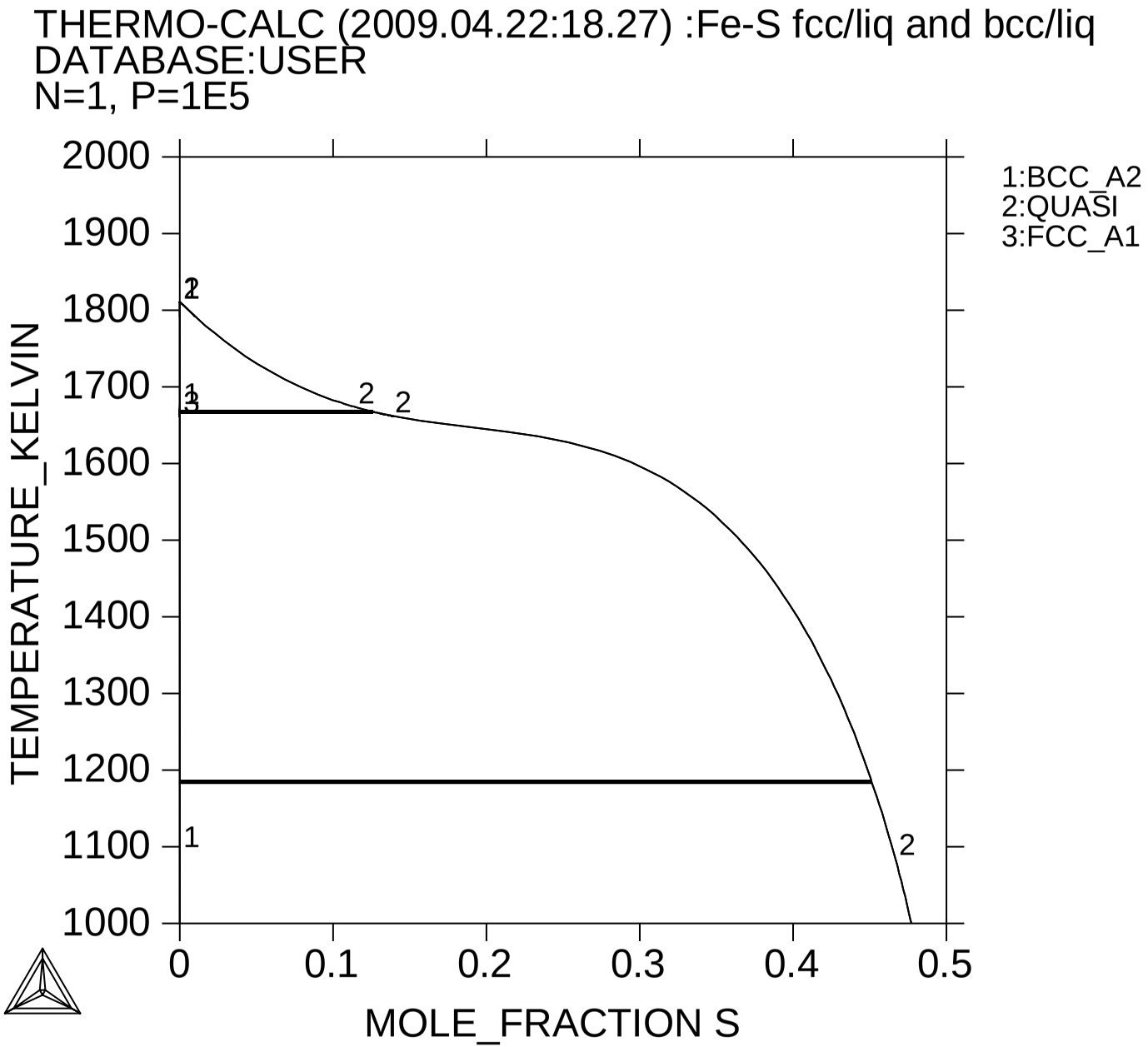
POST: set-title Fe-S fcc/liq and bcc/liq
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time          117  seconds
```

THERMO-CALC (2009.04.22:18.26) :log(gamma_S) in Fe-S liquid
DATABASE:USER
T=1873, P=1E5, N=1.;



THERMO-CALC (2009.04.22:18.26) :log(gamma_S)in Fe-S liquid
DATABASE:USER
T=2023, P=1E5, N=1.;




THERMO-CALC (2009.04.22:18.27) :Fe-S fcc/liq and bcc/liq
DATABASE:USER
N=1, P=1E5
TEMPERATURE_KELVIN
MOLE_FRACTION S
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
0
0.1
0.2
0.3
0.4
0.5
1:BCC_A2
2:QUASI
3:FCC_A1

51

Calculation of molar volume, thermal expansivity and density

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ This example shows calculations of volume, thermal expansivity
SYS: @@ and density
SYS:
SYS: set-log ex51,,
SYS:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: sw tcfe6
   ... the command in full is SWITCH_DATABASE
TDB_TCFE6:
TDB_TCFE6: @@ volume of a unary system
TDB_TCFE6: d-sys fe
   ... the command in full is DEFINE_SYSTEM
 FE  DEFINED
TDB_TCFE6: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  A1_KAPPA                KAPPA
 LAVES_PHASE_C14  REJECTED
TDB_TCFE6: rest-ph fcc,bcc,liq
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  LIQUID:L
   RESTORED
TDB_TCFE6: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
 -OK-
TDB_TCFE6:
TDB_TCFE6: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=400, n=1, p=1e5
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated           3  grid points in           0  s
POLY_3: s-a-v 1 t 298 2000,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: save tcex51 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
```

```
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    400.000
 Global calculation of initial equilibrium ....OK

 Phase Region from    400.000     for:
     BCC_A2
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
 Global check of adding phase at  1.18481E+03
 Calculated    81 equilibria

 Phase Region from    1184.81     for:
     BCC_A2
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    1184.81     for:
     FCC_A1
 Global test at  1.26000E+03 .... OK
 Global test at  1.36000E+03 .... OK
 Global test at  1.46000E+03 .... OK
 Global test at  1.56000E+03 .... OK
 Global test at  1.66000E+03 .... OK
 Global check of adding phase at  1.66747E+03
 Calculated    51 equilibria

 Phase Region from    1667.47     for:
     BCC_A2
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    1667.47     for:
     BCC_A2
 Global test at  1.74000E+03 .... OK
 Global check of adding phase at  1.81095E+03
 Calculated    18 equilibria

 Phase Region from    1810.95     for:
     LIQUID
     BCC_A2
 Calculated     2 equilibria

 Phase Region from    1810.95     for:
     LIQUID
 Global test at  1.89000E+03 .... OK
 Global test at  1.99000E+03 .... OK
 Terminating at    2000.00
 Calculated    22 equilibria

 Phase Region from    400.000     for:
     BCC_A2
 Global test at  3.20000E+02 .... OK
 Terminating at    298.000
 Calculated    14 equilibria
 *** Buffer saved on file: tcex51.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

POST: s-d-a x t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51a
POST: s-l e
```

```
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST: @@ define and plot density
POST: ent fun density=b*1e-3/vm;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y density
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-axis-text y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Density (kg/m3)
POST: set-title example 51b
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST: @@ define and plot coefficient of linear
POST: @@  thermal expansion
POST: ent fun alpha_bcc=vm(bcc).t/vm(bcc)/3;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y alpha_bcc
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-axis-text y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Thermal expansivity of bcc
POST: set-title example 51c
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST:@?
POST: back
POLY_3: @@ volume of Fe-C binary system
POLY_3: go d
   ... the command in full is GOTO_MODULE
TDB_TCFE6: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 IONIC_LIQ:Y            L12_FCC                B2_BCC
 B2_VACANCY             HIGH_SIGMA             DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
TDB_TCFE6: de-sys fe c
   ... the command in full is DEFINE_SYSTEM
 FE                     C  DEFINED
TDB_TCFE6: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L               BCC_A2                 FCC_A1
 HCP_A3                 DIAMOND_FCC_A4         GRAPHITE
 CEMENTITE              M23C6                  M7C3
 M5C2                   KSI_CARBIDE            A1_KAPPA
 KAPPA                  FE4N_LP1               FECN_CHI
 LAVES_PHASE_C14  REJECTED
TDB_TCFE6: res-ph fcc,bcc,cem,liq
   ... the command in full is RESTORE
 FCC_A1                 BCC_A2                 CEMENTITE
 LIQUID:L  RESTORED
TDB_TCFE6: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....
```

```
 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
  'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
      -FE'
  'B. Uhrenius (1993-1994), International journal of refractory metals and
      hard mater, Vol. 12, pp. 121-127; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
 -OK-
TDB_TCFE6:
TDB_TCFE6: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=400, n=1, p=1e5
   ... the command in full is SET_CONDITION
POLY_3: s-c w(c)=.6e-2
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          412  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: s-a-v 1 t 298 2000,,
   ... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: save tcex51 y
   ... the command in full is SAVE_WORKSPACES

 This file contains results from a previous STEP or MAP command.
 The SAVE command will save the current status of the program but destroy
 the results from the previous STEP or MAP commands.

POLY_3: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    400.000
 Global calculation of initial equilibrium ....OK

 Phase Region from    400.000     for:
     BCC_A2
     CEMENTITE
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global check of adding phase at  9.99783E+02
 Calculated    62 equilibria

 Phase Region from    999.783     for:
     BCC_A2
     CEMENTITE
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    999.783     for:
     BCC_A2
     FCC_A1
 Global check of removing phase at  1.02363E+03
 Calculated     6 equilibria

 Phase Region from    1023.63     for:
     FCC_A1
 Global test at  1.10000E+03 .... OK
 Global test at  1.20000E+03 .... OK
 Global test at  1.30000E+03 .... OK
 Global test at  1.40000E+03 .... OK
```

```
 Global test at  1.50000E+03 .... OK
 Global test at  1.60000E+03 .... OK
 Global check of adding phase at  1.69090E+03
 Calculated    70 equilibria

 Phase Region from    1690.90     for:
     LIQUID
     FCC_A1
 Global check of removing phase at  1.76294E+03
 Calculated    10 equilibria

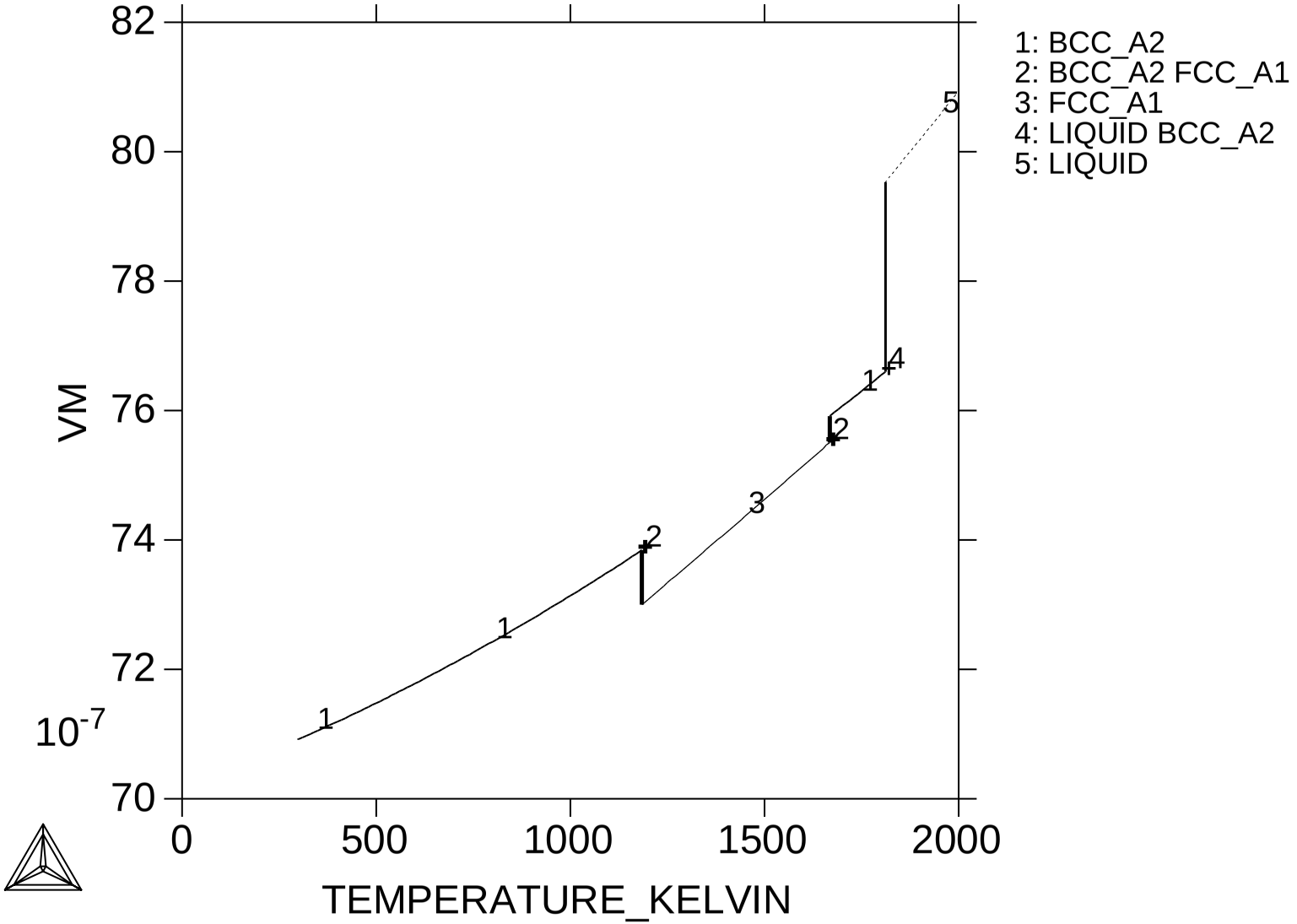
 Phase Region from    1762.94     for:
     LIQUID
 Global test at  1.84000E+03 .... OK
 Global test at  1.94000E+03 .... OK
 Terminating at    2000.00
 Calculated    27 equilibria

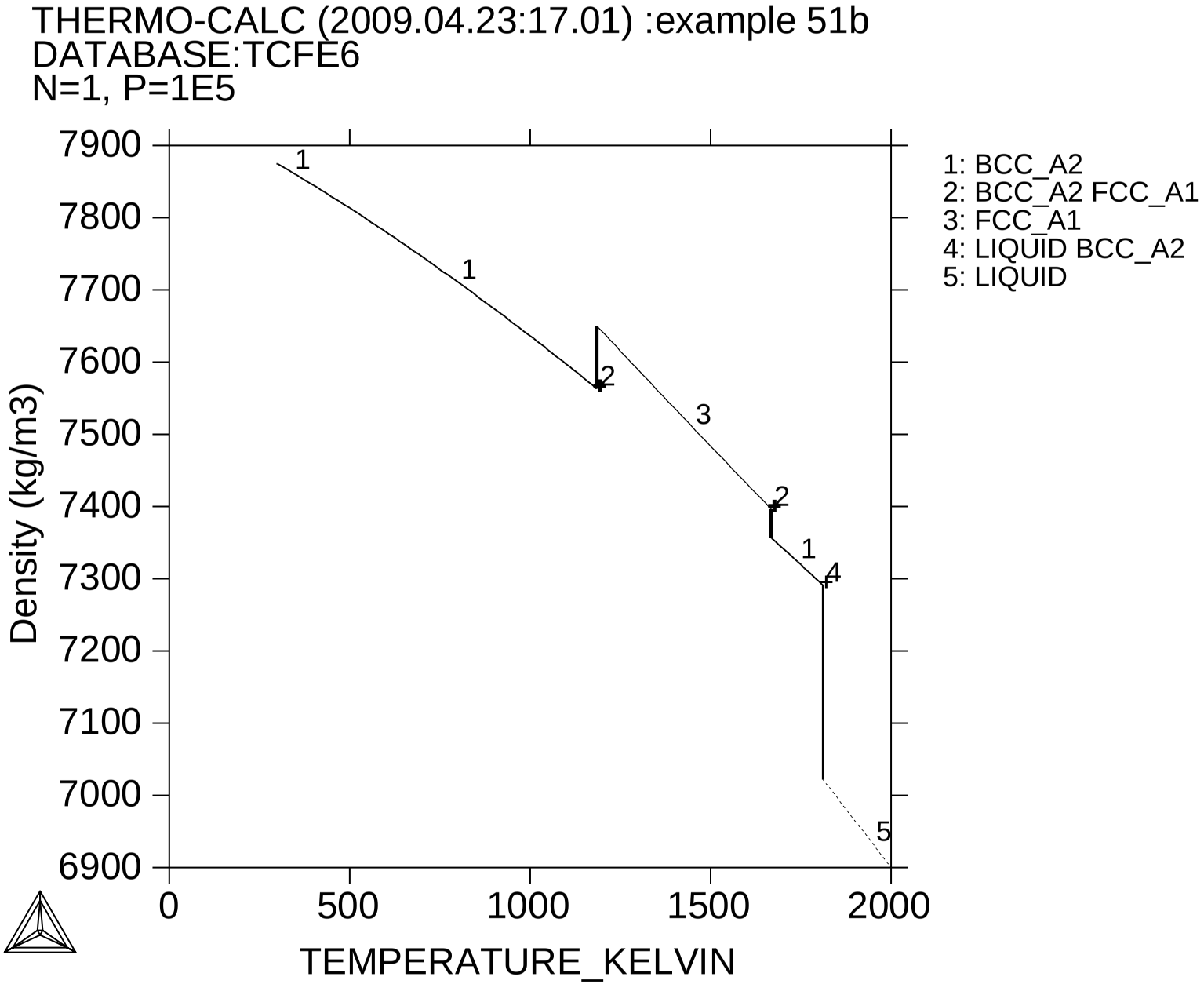
 Phase Region from    400.000     for:
     BCC_A2
     CEMENTITE
 Global test at  3.20000E+02 .... OK
 Terminating at    298.000
 Calculated    14 equilibria
 *** Buffer saved on file: tcex51.POLY3
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

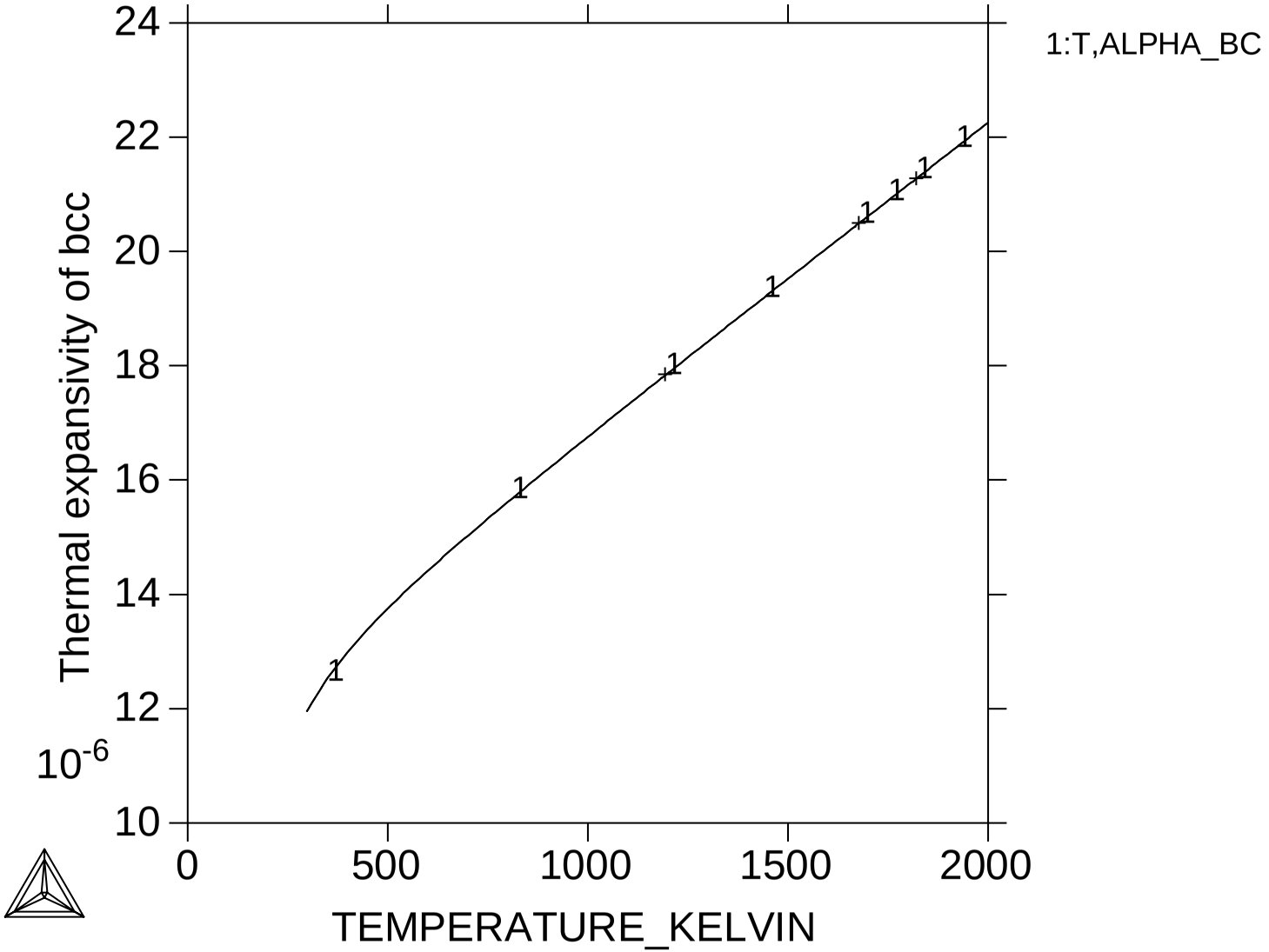
POST: s-d-a x t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51d
POST: s-l e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST:
POST: @?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST: CPU time           4  seconds
```

THERMO-CALC (2009.04.23:17.01) :example 51a
DATABASE:TCFE6
N=1, P=1E5

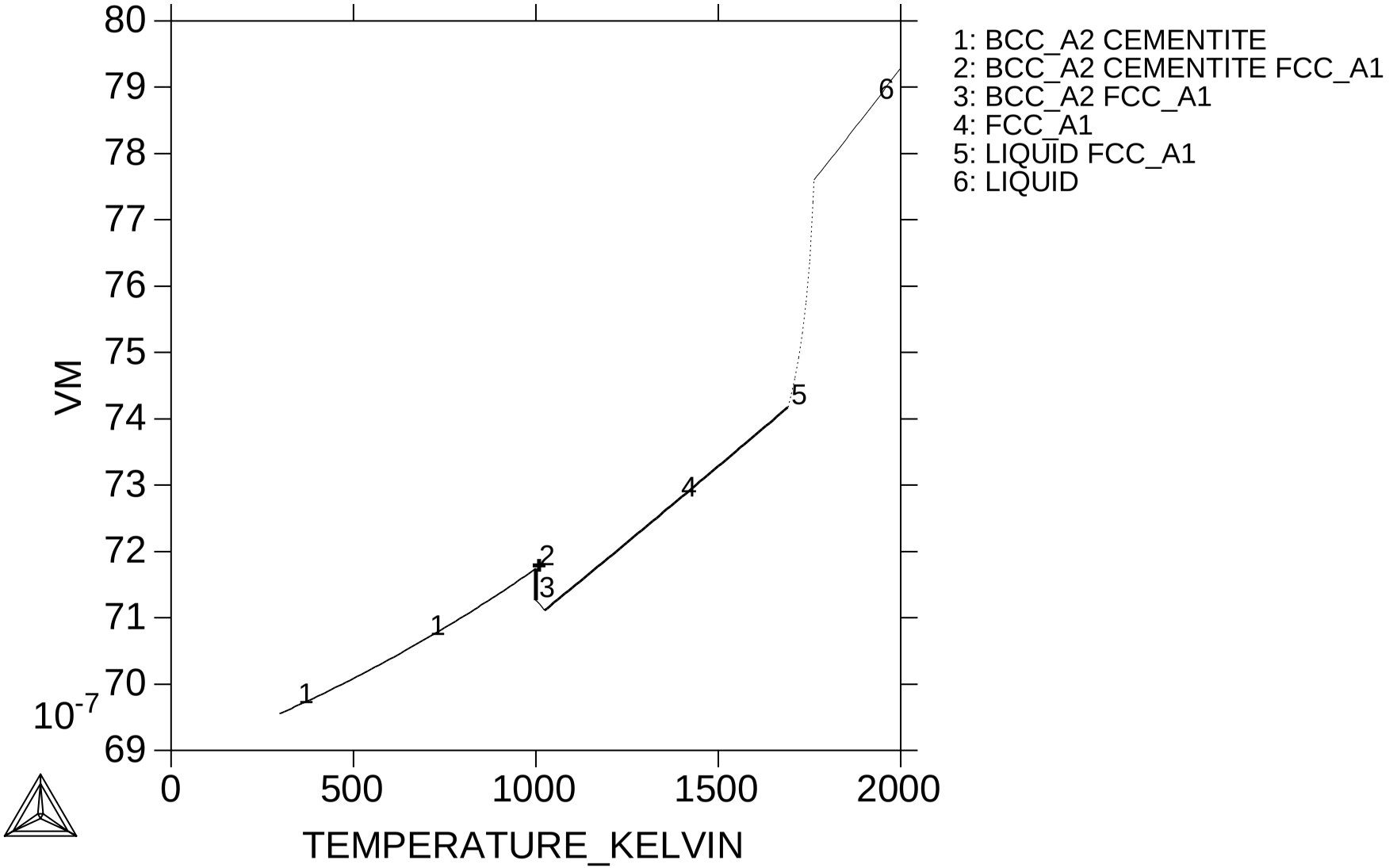



THERMO-CALC (2009.04.23:17.01) :example 51b
DATABASE:TCFE6
N=1, P=1E5
Density (kg/m3)
7900
7800
7700
7600
7500
7400
7300
7200
7100
7000
6900
0
500
1000
1500
2000
TEMPERATURE_KELVIN
1: BCC_A2
2: BCC_A2 FCC_A1
3: FCC_A1
4: LIQUID BCC_A2
5: LIQUID

THERMO-CALC (2009.04.23:17.01) :example 51c
DATABASE:TCFE6
N=1, P=1E5



THERMO-CALC (2009.04.23:17.01) :example 51d
DATABASE:TCFE6
N=1, P=1E5, W(C)=6E-3;



52

Changing the excess models for interaction parameters in a solution phase

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@
SYS: @@ ========================================================================
SYS: @@ Example showing how to change the excess models for binary/ternary
SYS: @@ interactions in a solution phase, either through direct interactive
SYS: @@ amendments of phase descriptions within the GES module, or enforced
SYS: @@ by specific type-definitions given in a database file retrieved by
SYS: @@ the TDB module.
SYS: @@  ----------------------------------------------------------------
SYS: @@   For Binary Excess Model:
SYS: @@           from the default R-K model   to Mixed-Excess-Model
SYS: @@                 (Note the phase has to be a substitutional phase)
SYS: @@  ----------------------------------------------------------------
SYS: @@   For Ternary Extrapolation Model:
SYS: @@           from the default R-K-M model to Toop_Kohler model
SYS: @@
SYS:
SYS: set-log TCEX52.LOG
Heading: Example showing how to enter a TOOP binary extrapolation model
SYS:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
TDB_TCFE6:
TDB_TCFE6: go gibbs
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM version  5.2
 First version released 1-Jan-78, last update 20-Nov-2007

GES:
GES: ent-el  /- VA A B C
   ... the command in full is ENTER_ELEMENT
GES:
GES: am_el_d /-  ELECTRON_GAS            0.0000E+00  0.0000E+00  0.0000E+00
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d VA  VACUUM                  0.0000E+00  0.0000E+00  0.0000E+00
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d A   UNKNOWN                 1.0000E+01  0.0000E+00  0.0000E+00
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d B   BETA_RHOMBO_B           1.0811E+01  1.2220E+00  5.9000E+00
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d C   GRAPHITE                1.2011E+01  1.0540E+00  5.7400E+00
   ... the command in full is AMEND_ELEMENT_DATA
GES:
GES: ent-phase LIQUID  L,  1   A,B,C ;  N N
   ... the command in full is ENTER_PHASE
GES:
GES: ent-param G(LIQUID,A;0) 298.15 0; 6000 N!
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A;0)-H298(UNKNOWN,A;0)
GES: ent-param G(LIQUID,B;0) 298.15 0; 6000 N!
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0)
GES: ent-param G(LIQUID,C;0) 298.15 0; 6000 N!
```

```
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,C;0)-H298(GRAPHITE,C;0)
GES:
GES: ent-param L(LIQUID,A,B;0)  298.15  10000;  6000 N
   ... the command in full is ENTER_PARAMETER
 L(LIQUID,A,B;0)
GES: ent-param L(LIQUID,A,B;1)  298.15 -10000;  6000 N
   ... the command in full is ENTER_PARAMETER
 L(LIQUID,A,B;1)
GES:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH          DATE 2009- 4-23
 FROM DATABASE: UNKNOWN

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00

 SPECIES                                    STOICHIOMETRY
   1 A                                      A
   2 B                                      B
   3 C                                      C
   4 VA                                     VA

 Sorry, no data output from this database

 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE

GES: @?<Hit_return_to_continue>
GES:
GES: @@
GES: @@ First Step: Amending the binary excess model:
GES: @@ ********** ======================================================
GES: @@ The default binary excess model is the Redlich-Kister Model for all
GES: @@  the three associated binary interaction pairs (A-B, A-C and B-C)
GES: @@  in the substitutional LIQUID solution phase (without sublattice)
GES: @@  that consists of three elements (A, B and C).
GES: @@
GES: @@ Before changing this default binary excess model for the ternary
GES: @@  LIQUID solution phase, one must have already entered the G
GES: @@  parameters (for standard Gibbs energies of all pure end-members)
GES: @@  and L parameters (for binary R-K excess interaction energies),
GES: @@  as shown here!
GES: @@
GES: @@ In this particular example, we want to change from the default R-K
GES: @@  binary excess model to the Mixed-Excess-Model (with three different
GES: @@  binary excess models, namely Legendre, Polynom and Redlich-Kister
GES: @@  models, applied to the A-B, A-C and B-C binaries, respectively),
GES: @@  as demonstrated below:
GES: @@
GES:
GES: @@... For the A-B interaction, the Legendre binary excess model should
GES: @@      be used (rather than the default Redlich-Kister Model), with
GES: @@      the first species (i.e. A) as the independent constituent
GES: @@      and the second species (i.e. B) as the dependent constituent,
GES: @@      while the L parameters for the A-B interaction shall remain
GES: @@      the same as those handled by the R-K model.
GES: @@
GES: amend-phase-description liquid
AMEND WHAT /COMPOSITION_SETS/:  ?
```

```
 You can amend
 EXCESS_MODEL
 MAGNETIC_ORDERING
 DEBYE_HUCKEL
 STATUS_BITS
 NEW_CONSTITUENT
 RENAME_PHASE
 COMPOSITION_SETS
 GLASS_TRANSITION
 DISORDERED_PART
 MAJOR_CONSTITUENT
 ZRO2_TRANSITION
 REMOVE_ADDITIONS
 QUASICHEM_IONIC
 QUASICHEM_FACT00
 QUASICHEM_IRSID
 TERNARY_EXTRAPOLAT
 HKF_ELECTROSTATIC
 DEFAULT_STABLE
 SITE_RATIOS
 FRACTION_LIMITS
AMEND WHAT /COMPOSITION_SETS/: excess
MODEL NAME /REDLICH-KISTER_MUGGIANU/: ?
 REDLICH-KISTER_MUGGIANU
 REDLICH-KISTER_KOHLER
 FLORY-HUGGINS POLYMER MODEL
 MIXED-EXCESS-MODELS (R-K default)
 HKF
 PITZER
 CENTRAL_ATOM_MODEL

MODEL NAME /REDLICH-KISTER_MUGGIANU/: mixed
First (the independent) constituent: ?
 First (the independent) constituent

  Specify the first (the independent) constituent of a certain binary pair
  of constituents in the current substitutional solution phase, for which you
  wish to change the binary excess model from the default REDLICH-KISTER
  model to another model (LEGENDRE or POLYNOM). This sub-option will be
  repeatedly prompted (again and again), after having specified the desired
  binary Excess model type, for further changes of binary excess model for
  other specific binary pair in the current substitutional solution phase.

  By simply typing <RETURN> at such a repeated prompt (implying that there
  will be no more changes of binary excess model for all other possibly-
  remaining binary pairs that shall still use the default REDLICH-KISTER
  model), you can finish this MIXED-EXCESS-MODELS option.

First (the independent) constituent: A
Second (the dependent) constituent: B
Excess model type: /LEGENDRE/: ?
Legal choices are: LEGENDRE, POLYNOM or REDLICH-KISTER
Excess model type: /LEGENDRE/: legendre
 Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent: NONE
GES:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH          DATE 2009- 4-23
 FROM DATABASE:

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00

 SPECIES                                  STOICHIOMETRY
   1 A                                    A
```

```
  2 B                                     B
  3 C                                     C
  4 VA                                    VA

 Sorry, no data output from this database

 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE
```

GES: **@?<Hit_return_to_continue>**

```
GES:
```

GES: ***@@... For the A-C interaction, the Polynom binary excess model should***
GES: ***@@ be used (rather than the default Redlich-Kister Model), with***
GES: ***@@ the second species (i.e. C) as the independent constituent***
GES: ***@@ and the first species (i.e. A) as the dependent constituent,***
GES: ***@@ while the L parameters for the A-C interaction shall remain***
GES: ***@@ the same as those handled by the R-K model.***
GES: *@@*

GES: **ent-param G(LIQUID,A,C;0) 298.15 10000; 6000 N**

```
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A,C;0)
```

GES: **ent-param G(LIQUID,A,C;1) 298.15 5000; 6000 N**

```
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A,C;1)
```

GES:

GES: **amend-phase-des LIQUID excess mixed C A polynom**

```
   ... the command in full is AMEND_PHASE_DESCRIPTION

 Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent:
```

GES: **list-data ,,**

```
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH           DATE 2009- 4-23
 FROM DATABASE:

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00

 SPECIES                                  STOICHIOMETRY
   1 A                                    A
   2 B                                    B
   3 C                                    C
   4 VA                                   VA

 Sorry, no data output from this database

 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE
```

GES: **@?<Hit_return_to_continue>**

```
GES:
```

GES: ***@@... For the B-C interaction, the default Redlich-Kister binary***
GES: ***@@ excess model shall still be used; so we do not need to amend***
GES: ***@@ anything regarding that.***
GES: *@@*

GES: **ent-param G(LIQUID,B,C;0) 298.15 10000; 6000 N**

```
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,B,C;0)
GES: ent-param G(LIQUID,B,C;1)  298.15 -2000;  6000 N
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,B,C;1)
GES:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH          DATE 2009- 4-23
 FROM DATABASE:

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00

 SPECIES                                    STOICHIOMETRY
   1 A                                      A
   2 B                                      B
   3 C                                      C
   4 VA                                     VA

 Sorry, no data output from this database

 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE

GES: @?<Hit_return_to_continue>
GES:
GES: @@
GES: @@Second Step: Amending the ternary extrapolation model:
GES: @@********** ==========================================================
GES: @@The default ternary excess model is the Redlich-Kister_Muggianu
GES: @@ Model (i.e., the MUGGIANU_RESTOR method for ternary extrapolation
GES: @@ based on binary parameters) for the associated ternary interaction
GES: @@ terms; when no ternary L parameter is entered for that, such a
GES: @@ default Redlich-Kister_Muggianu Model is thus to be used for
GES: @@ extrapolation from binary excess energies to ternary interactions
GES: @@ in the substitutional LIQUID solution phase (without sublattice)
GES: @@ that consists of three elements (A, B and C).
GES: @@
GES: @@However, in this particular example as illustrated in the following,
GES: @@ we shall change from this default R-K-M ternary excess model to
GES: @@ the TOOP-KOHLER method for the ternary extrapolation method, with
GES: @@ the species C as the Toop constituent, while the species A and B
GES: @@ as the Kohler constituents (entering A and B, or B and A, as the
GES: @@ basis constituent and first interacting constituent). This will
GES: @@ implicitly enforce that, during the ternary extrapolation, only
GES: @@ the A-B binary interaction parameters are utilized in accordance
GES: @@ with the Kohler ternary extrapolation formula for A-B-C ternary
GES: @@ interaction, while any other binary interaction parameters
GES: @@ involving the Toop species C (i.e., of A-C and B-C binaries) are
GES: @@ used in line with the Toop-Kohler ternary extrapolation formula
GES: @@ (for the A-C-B and B-C-A ternary interactions). This makes the
GES: @@ extrapolated ternary excess interaction terms different from
GES: @@ those handled either by the default MUGGIANU_RESTOR method
GES: @@ or by the alternative KOHLER-ALL method.
GES: @@
GES: @@Note that only when all the relevant binary excess energies in a
GES: @@ ternary system are treated by the default Redlich-Kister Model
GES: @@ (i.e., the Mixed-Excess-Model should have not been used), the
GES: @@ MUGGIANU_RESTOR method for ternary extrapolations is equivalent
GES: @@ to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method
```

```
GES: @@ to the Redlich-Kister_Kohler Model.
GES: @@
GES: amend_phase-des LIQUID
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/:  ?
 You can amend
 EXCESS_MODEL
 MAGNETIC_ORDERING
 DEBYE_HUCKEL
 STATUS_BITS
 NEW_CONSTITUENT
 RENAME_PHASE
 COMPOSITION_SETS
 GLASS_TRANSITION
 DISORDERED_PART
 MAJOR_CONSTITUENT
 ZRO2_TRANSITION
 REMOVE_ADDITIONS
 QUASICHEM_IONIC
 QUASICHEM_FACT00
 QUASICHEM_IRSID
 TERNARY_EXTRAPOLAT
 HKF_ELECTROSTATIC
 DEFAULT_STABLE
 SITE_RATIOS
 FRACTION_LIMITS
AMEND WHAT /COMPOSITION_SETS/:  TERN-EXT
Extrapolation method: /TOOP-KOHLER/:  ?
 Default method is Muggianu, you can use
 TOOP-KOHLER
 KOHLER-ALL
 MUGGIANU_RESTOR
Extrapolation method: /TOOP-KOHLER/:  TOOP-KOHLER
Constituent in sublattice 1: A
First interaction constituent: B
Toop constituent: C
GES:
GES: list-data ,,
 Sorry, LIST-DATA disabled for this database

1OUTPUT FROM GIBBS ENERGY SYSTEM ON UNIX / KTH           DATE 2009- 4-23
 FROM DATABASE:

 ALL DATA IN SI UNITS
 FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00
  1 A    UNKNOWN                   1.0000E+01  0.0000E+00  0.0000E+00
  2 B    BETA_RHOMBO_B             1.0811E+01  1.2220E+00  5.9000E+00
  3 C    GRAPHITE                  1.2011E+01  1.0540E+00  5.7400E+00

 SPECIES                                   STOICHIOMETRY
   1 A                                     A
   2 B                                     B
   3 C                                     C
   4 VA                                    VA

 Sorry, no data output from this database

 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C
 No data listing for this database

 LIST_OF_REFERENCES
 NUMBER  SOURCE

GES: @?<Hit_return_to_continue>
GES:
GES: @@ Third Step: Performing an equilibrium calculation
GES: @@               using the entered and amended descriptions.
GES: @@ ********** ==========================================================
```

```
GES: @@
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e , X
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database:

 Conditions:
 T=1500, P=1E5, N=1, X(B)=0.2, X(C)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1500.00 K (  1226.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.07655E+01
 Total Gibbs energy -9.98602E+03,  Enthalpy  2.85557E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       5.0000E-01  5.0000E-01 4.7833E-01 -9.1973E+03 SER
 B                       2.0000E-01  2.0000E-01 1.9875E-01 -2.0151E+04 SER
 C                       3.0000E-01  3.0000E-01 5.5332E-01 -7.3811E+03 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0765E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.00000E-01  C  3.00000E-01  B  2.00000E-01
POLY_3: sh qf(*)
   ... the command in full is SHOW_VALUE
 QF(LIQUID)=0.59180178
POLY_3: sh gm(*) dgm(*)
   ... the command in full is SHOW_VALUE
 GM(LIQUID)=-9986.019
 DGM(LIQUID)=0
POLY_3:
POLY_3: save TCEX52a.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: @@ Fourth Step: Reading the same data from a small database and
POLY_3: @@              Performing the same equilibrium calculation.
POLY_3: @@ ************ ========================================================
POLY_3: @@
POLY_3: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE6: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
TDB_TCFE6:
TDB_TCFE6: sw user TCEX52-TOOP.TDB
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
TDB_USER: d-sys /all
   ... the command in full is DEFINE_SYSTEM
 A                       B                       C
   DEFINED
TDB_USER: l-sys const
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :A B C:
TDB_USER: get
   ... the command in full is GET_DATA
```

```
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Reference 2'
  'Reference 1'
 AFTER ...
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 -OK-
TDB_USER:
TDB_USER: @?<Hit_return_to_continue>
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3:
POLY_3: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
   ... the command in full is SET_CONDITION
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         1977  grid points in            0  s
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e , X
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1500, P=1E5, N=1, X(B)=0.2, X(C)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1500.00 K (  1226.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.07655E+01
 Total Gibbs energy -9.98602E+03,  Enthalpy  2.85557E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       5.0000E-01  5.0000E-01 4.7833E-01 -9.1973E+03 SER
 B                       2.0000E-01  2.0000E-01 1.9875E-01 -2.0151E+04 SER
 C                       3.0000E-01  3.0000E-01 5.5332E-01 -7.3811E+03 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0765E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.00000E-01  C  3.00000E-01  B  2.00000E-01
POLY_3: sh qf(*)
   ... the command in full is SHOW_VALUE
 QF(LIQUID)=0.59180178
POLY_3: sh gm(*) dgm(*)
   ... the command in full is SHOW_VALUE
 GM(LIQUID)=-9986.019
 DGM(LIQUID)=0
POLY_3:
POLY_3: save TCEX52b.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: @@
POLY_3: @@ As you have noticed above, the calculated equilibrium (using the
POLY_3: @@   small database) is exactly the same as the first calculation
POLY_3: @@   (with data amended in the GES module step-by-step, for the
POLY_3: @@   binary/ternary excess models).
POLY_3: @@
POLY_3:
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: set-inter
   ... the command in full is SET_INTERACTIVE
POLY_3: CPU time           0  seconds
```

53

Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine

```
 Thermo-Calc version S(build 1584) on Linux
 Copyright (1993,2008) Foundation for Computational Thermodynamics,
 Stockholm, Sweden
 Double precision version linked at 16-03-09 10:23:29
 Only for use at TCSAB internal
 Local contact Annica
SYS:SYS:SYS:SYS:SYS:SYS:SYS:SYS: @@
SYS: @@ TCEX53: TCCS (Thermo-Calc Classic,Version S) Standard Example No 53
SYS: @@ ******* ============================================================
SYS: @@   Copyright: Thermo-Calc Software AB, Stockholm, Sweden
SYS: @@   Date:      2008-4-18
SYS: @@
SYS: @@ Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine
SYS: @@ ********************************************************************
SYS: @@    * Using PAQ2 or PAQS2 database;
SYS: @@    * For the Fe-X-H2O-NaCl heterogeneous interaction systems
SYS: @@              (X = Cr-Ni-Co)
SYS: @@ ============================================================================
SYS: @@ Note: The PAQ2 (TCS Public Aqueous Solution (SIT) Database, v2.4;
SYS: @@         using the SIT aqueous solution model) or PAQS2 (TCS Public
SYS: @@         Aqueous Solution Database, v2.4; using the Complete Revised
SYS: @@         HKF aqueous solution model) contains an AQUEOUS solution
SYS: @@         phase and REF_ELECTRODE phase (as a reference for electron
SYS: @@         in aqueous electrolyte systems), as well as some data for
SYS: @@         various solid phases (solution or stoichiometric) and
SYS: @@         gaseous mixture phase. Therefore, it can be used, via the
SYS: @@         Single-Database Option in the POURBAIX module or through
SYS: @@         the normal TDB-GES-PLOY-POST routine, for calculations of
SYS: @@         the so-called Pourbaix diagrams (i.e., Eh-pH plots) and
SYS: @@         other types of diagrams in aqueous-bearing multicomponent
SYS: @@         heterogeneous interaction systems.
SYS: @@ ----------------------------------------------------------------------
SYS: @@ Also Note: The initial bulk compositions of Fe-based alloys in these
SYS: @@              testing calculations are just preliminarily assigned,
SYS: @@              in which the BCC_A2 and/or FCC_A1 solution phase(s) are
SYS: @@              considered as of primarily interest.
SYS: @@            For precise calculations, one shall have more practical
SYS: @@              inputs for the initial bulk compositions of alloys.
SYS: @@ ----------------------------------------------------------------------
SYS: @@
SYS: go sys
SYS:
SYS:
SYS: set-log TCEX53.LOG
Heading: Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine
SYS:
SYS: @@ ============================================================================
SYS: @@ Step 1: Single-Point Calculations for H2O-NaCl system
SYS: @@ ********************************************************************
SYS: @@   To demonstrate how to define the molality of NaCl
SYS: @@       in an aqueous-bearing heterogeneous interaction system
SYS: @@
SYS:
SYS: @@... Retrieving data from the PAQ2 or PAQS2 database:
SYS: go d
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module running on UNIX / KTH
 Current database: TCS Steels/Fe-Alloys Database v6

 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
TDB_TCFE6: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 IONIC_LIQ:Y             L12_FCC                 B2_BCC
 B2_VACANCY              HIGH_SIGMA              DICTRA_FCC_A1
   REJECTED
 REINITIATING GES5 .....
TDB_TCFE6: @@ ------ switch on PAQ2 or PAQS2
TDB_TCFE6: sw PAQ2
   ... the command in full is SWITCH_DATABASE
```

Current database: TCS Public Aqueous Soln (SIT) TDB v2

H	O	ZE
VA DEFINED		
LIQUID:L REJECTED		
GRAPHITE	DIAMOND_A4	FC_ORTHORHOMBIC
MONOCLINIC REJECTED		
CBCC_A12	CUB_A13	CHI_A12
FE4N	FECN_CHI REJECTED	
CEMENTITE	M23C6	M7C3
M5C2	M3C2	KSI_CARBIDE
PI REJECTED		
FE3C	NI3C	CR3C2
CR7C3	CR23C6 REJECTED	
COCO3	FECO3	NAHCO3
NA2CO3	NA2CO3_S2	NICO3
CRC6O6 REJECTED		
CO3N	CRN	CR2N
FE2N	NI3N REJECTED	
NANO2	NANO2_S2	NANO3
REJECTED		
COCL2	CRCL2	CRCL3
FECL2	FECL3	NICL2
REJECTED		
FECLO	NACLO4	NACLO4_S2
REJECTED		

TDB_PAQ2: **data**

... the command in full is DATABASE_INFORMATION

Current database: TCS Public Aqueous Soln (SIT) TDB v2

PAQ2

Thermo-Calc PUBLIC AQUEOUS DATABASE FOR POURBAIX MODULE

(based on and replacing AQ in TCC/TCW & PAQ in TCC-Demo/TCW-Demo)

****

(Version 2.4, Feb. 2008)

Copyright @ 1997-2008: Thermo-Calc Software AB, Sweden

This public aqueous solution database contains aqueous solution species, and gaseous mixture species and solid/liquid (pure and solution) phases in an 11-element system (Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl). As a demo version of the complete TCAQ2 Aqueous Solution Database, it is specially designed for uses with the apecial POURBAIX module which allows easy and automatic calculations of the sp-called Pourbaix diagrams (i.e., Eh-pH plots) and many types of property diagrams. It can also be used in normal TCC/TCW calculations for aqueous involved hetergeneous interaction systems.

The TCAQ2 Aqueous Solution Database covers 83 elements (compatible with the SGTE PURE/SSUB/SSOL and other databases), and can be used together with the SIT (Specific Interaction Theory) Model for complex aqueous solution that has already implemented in Thermo-Calc.

PAQ has been developed since 1996, and gradually modified and expanded later on. PAQ2.4 combines 4 files from its previous version PAQ2 [i.e., PAQ2setup.TDB for defining elements, species and phases; PAQ2param.TDB for assigning various functions and parameters for standard properties of various phases; PAQ2inter.TDB for assigning binary or higher-order interaction parameters for non-ideal properties of aqueous solution phase; and PAQ2funct.TDB for entering extra functions referred in PAQ2param.TDB].

The AQUEOUS solution phase can be treated by the SIT Model, using the TCAQ2 (or PAQ2) database that can be applied to low PTX conditions (up to 100 bar, 350 C and 3 molality). However, if investigated hetergeneous interaction processes occur at high PTX (up to 5 kbar, 1000 C and 10 molality), the other aqueous solution database, called AQS2, which implies the complete Revised HKF (Helgeson-Kirkham-Flowers) Model, is required.

Data for pure elements are taken from the SGTE unary database (PURE) with explicit magnetic and pressure dependencies. The reference state is 298.15 K and 1 bar. All data follow the new temperature scale ITPS 90.

For calculations of the so-called Pourbaix-diagrams (pH-Eh) and related

property diagrams within either the POURBAIX-module or through normal TDB-GES-POLY-POST routines, following types of phases must be defined in the heterogeneous interaction systems:

```
  AQUEOUS:        from PAQ2 (or PAQS2) or TCAQ2 (or AQS2);
  REF_ELECTRODE:  from PAQ2 (or PAQS2) or TCAQ2 (or AQS2);
  GAS:            from PAQ2 (or PAQS2) or SSUB4 (or TCMP2);
  Various Solids: from PAQ2 (or PAQS2) or SSOL4 (or TCFE6, TCMP2, etc.).
```

There are many solid phases (stoichiometric or solution) and a metallic liquid mixture phase which are included in the public PAQ2 and PAQS2 databases. By default, however, many such phases have been rejected automatically. Of course, if one wishes to consider any of such phases (such as Cementite or M23C6) into a defined interaction system, they can be appropriately restored in the POURBAIX or TDB modules.

Either TCAQ2 or AQS2 databases can be used by the advanced, easy-to-use POURBAIX Module via its multiple-database option, or be utilized along with ordinary Thermo-Calc routines. For a gaseous mixture phase, one could append from the SSUB (SGTE PURE SUBSTANCES DATABASE, which treats the gas phase as an ideal mixture at all temperatures, pressures and compositions), or from some non-ideal gaseous/fluid mixture models implemented in the Thermo-Calc GES system (such as the SUPERFLUID model, i.e., the non-ideal EOS and non-ideal mixing for the C-H-O-S-N-Ar fluids; Shi and Saxena, 1992). For other condensed materials except for aqueous solution species, one could append data (of stoichiometric and solution solid phases) from any compatible Thermo-Calc database(s) [e.g., PURE, SSUB, SSOL, TCFE, TCNI, TCNF, CCC1, TTNi, TTTi, TTAl, TTMg, TTZr, NSLD, SEMC, TCMP, TCES, SALT, ION, SLAG, NOX, NUOX, SNUX, NUMT, GCE, and other substances/solutions databases), depending upon application systems and investigated aqueous-bearing heterogeneous interaction processes.

In a normal POLY calculation (single points, stepping, and/or mapping), one should always remember as the first step to appropriately redefine the components as follows:

```
   DEF-COMP H2O H+1 Ze Fe Ni NaCl Cl-1 S <& other components> ;
```

Then, one can appropriately define the equilibrium conditions, e.g.,

```
   SET-COND P=1e5 T=300 B=1000 N(H+1)=0 N(Ze)=0 N(Fe)=1e-6 N(NaCl)=3...;
```

and set the necessary reference states for some components, e.g.,

```
   SET-REFERENCE-STATE H2O AQUEOUS * 1E5 ;
   SET-REFERENCE-STATE ZE REF_ELEC * 1E5 ;
   SET-REFERENCE-STATE NaCl HALITE * 1E5 ;
   SET-REFERENCE-STATE Fe BCC * 1E5 ;
```

The pH and Eh are thus defined by entering the following functions:

```
   ENT-SYM FUNC pH=-log10(ACR(H+1)) ;
   ENT-SYM FUNC Eh=MUR(ZE)/RNF ;
```

However, if the reference state for H+1 component has been defined by

```
   SET-REFERENCE-STATE H+1 AQUEOUS * 1E5 ;
```

then the pH quantity should be alternatively entered as:

```
   ENT-SYM FUNC pH=-log10(ACR(H+1,AQUEOUS)) ;
```

For defining activity and activity coefficients of the solvent, use:

```
   ENT-SYM FUNC ACRH2O=ACR(H2O,AQUEOUS) ;
   ENT-SYM FUNC RCH2O=ACR(H2O,AQUEOUS) ;
```

while for defining activity, activity coefficients and molality of a specific solute species "i", use:

```
   ENT-SYM FUNC AIi=ACR(i,AQUEOUS)*AH2O ;
   ENT-SYM FUNC RCi=ACR(i,AQUEOUS)*YH2O/Y(AQUEOUS,i) ;
   ENT-SYM FUNC MLi=Y(AQUEOUS,i)*AH2O/YH2O ;
```

where RNF=96485.309, AH2O=55.508435 and YH2O=Y(AQUEOUS,H2O) as predefined functions, and i=Fe+2 (for instance) as species name.

Important Note: The REF_ELECTRODE phase is the reference electrode which should always be included in a defined system involving aqueous solution for the purpose of calculating electron potentail [MUR(ZE)], while this phase should always be SUSPENDED in all the POLY calculations.

For further information, please contact Dr. Pingfang Shi at TCSAB.

Release History:

Version 1.0	initial release (as AQ),	1997
Version 1.1	with minor improvements (as AQ),	1998
Version 1.2	with minor improvements (as AQ),	2000
Version 2.0	with major improvements (as PAQ2.0),	2002
Version 2.1	with minor improvements (as PAQ2.1),	2003
Version 2.2	with minor improvements (as PAQ2.2),	2006
Version 2.3	with minor improvements (as PAQ2.3),	2007

Version 2.4 with major improvements (as PAQ2.4), 2008

Edited by: Dr. Pingfang Shi (Thermo-Calc Software, 1997-2008).
==========

TDB_PAQ2: **d-sys H O Na Cl**
... the command in full is DEFINE_SYSTEM
NA CL DEFINED
TDB_PAQ2: **l-sys const**
... the command in full is LIST_SYSTEM
AQUEOUS:A :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CL2 CL-1 CLO2 CLO-1 CLO2-1
CLO3-1 CLO4-1 HCLO HCLO2 NA+1:
> Aqueous Solution: using the SIT Model (from TCAQ2 database)
REF_ELECTRODE :ZE:
> Reference Electrode for ZE potentail; always SUSPENDED in POLY.
GAS:G :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1NA1 CL2NA2 CL3NA3 H
H1NA1 H1NA1O1 H1O1 H1O2 H2 H2NA2O2 H2O1 H2O2 NA NA1O1 NA2 NA2O1 NA2O2 O O2
O3:
> Gaseous Mixture, using the ideal gas model
FCC_A1 :NA O:VA:
> This is also the MX (X=C,N) solution phase.
BCC_A2 :NA O:VA:
> This is also the MX3 (X=C,N) solution phase.
HCP_A3 :NA:VA:
> This is also the M2X (X=C,N) solution phase.
HALITE :NA1CL1:
NAO2 :NA1O2:
NA2O :NA2O1:
NA2O_S2 :NA2O1:
NA2O_S3 :NA2O1:
NA2O2 :NA2O2:
NA2O2_S2 :NA2O2:
NAOH :H1NA1O1:
NAOH_S2 :H1NA1O1:
TDB_PAQ2: **get**
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES ......
PHASES ....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
-Cl system.'
'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
-Na-Ni-C-H-O-N-S-Cl system.'
'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
from TCAQ2 which covers totally 83 elements and contains many more
aqueous solution species.'
-OK-
TDB_PAQ2: **@?<Hit_return_to_continue>**
TDB_PAQ2:
TDB_PAQ2: ***@@... Defining system-components and their proper reference states:***
TDB_PAQ2: **go p-3**
... the command in full is GOTO_MODULE

POLY version 3.32, Dec 2007
POLY_3: **d-com H2O H+1 ZE Na Cl**
... the command in full is DEFINE_COMPONENTS
POLY_3: **s-r-s H2O AQUEOUS * 1e5**
... the command in full is SET_REFERENCE_STATE

```
POLY_3: s-r-s Ze  REF_ELE * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT              STATUS    REF. STATE     T(K)          P(Pa)
 VA                     ENTERED   SER
 H2O                    ENTERED   AQUEOUS        *             100000
 H+1                    ENTERED   SER
 ZE                     ENTERED   REF_ELECTRODE  *             100000
 NA                     ENTERED   SER
 CL                     ENTERED   SER
POLY_3:
POLY_3: @@... One may turn off the Global Minimization in the calculations:
POLY_3: @@ AD_OP E_C n y 5000 y y 0 y 3 n ,,
POLY_3:
POLY_3: @@... Defining the equilibrium conditions:
POLY_3: @@    ------------------------------------------------------------
POLY_3: @@     Defining P-T and bulk composition in the interaction system
POLY_3: @@     for the calculations of initial equilibria:
POLY_3: @@
POLY_3: s-c p=1e5 t=298.15 B(H2O)=1000
   ... the command in full is SET_CONDITION
POLY_3: s-in-am b(Na1Cl1)=5
   ... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-c n(H+1)=0 n(Ze)=0
   ... the command in full is SET_CONDITION
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
    N(ZE)=0
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: @@... Calculating an initial equilibrium with only AQUEOUS presented:
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 AQUEOUS                ENTERED    0.00000000E+00  1.78560000E+03
 SUSPENDED PHASES:
 REF_ELECTRODE NAOH_S2 NAOH NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O HCP_A3
 HALITE FCC_A1 BCC_A2 GAS
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated           87  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
    N(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.56795E+01,  Mass in grams  1.00500E+03
 Total Gibbs energy -1.70630E+07,  Enthalpy -1.59010E+07,  Volume  0.00000E+00

 Component              Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                    5.5508E+01  9.9693E-01 9.9654E-01 -8.5871E+00 AQUEOUS
 H+1                   -9.7239E-08 -1.7464E-09 1.0405E-07 -3.9858E+04 SER
 ZE                     8.6043E-08  1.5453E-09 3.4476E+12  7.1565E+04 REF_ELEC
 NA                     8.5554E-02  1.5365E-03 4.5046E-63 -3.5588E+05 SER
 CL                     8.5554E-02  1.5365E-03 4.1623E-18 -9.9210E+04 SER

 AQUEOUS                    Status ENTERED     Driving force  0.0000E+00
 Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00  Mole fractions:
```

```
 H2O  9.96927E-01  NA   1.53654E-03  H+1 -1.74641E-09
 CL   1.53654E-03  ZE   1.54532E-09
 Constitution:           SiteFraction    Molality      Activity      log10Act
 H2O                     9.96927E-01   5.55084E+01   9.96605E-01    -0.0015
 CL-1                    1.53654E-03   8.55538E-02   6.73425E-02    -1.1717
 NA+1                    1.53654E-03   8.55538E-02   6.73424E-02    -1.1717
 H+1                     2.37132E-09   1.32034E-07   1.04050E-07    -6.9828
 OH-1                    2.19965E-09   1.22476E-07   9.63757E-08    -7.0160
 O2                      4.70269E-10   2.61844E-08   2.61828E-08    -7.5820
 O3                      1.00000E-12   0.00000E+00   2.70935E-38   -37.5671
 HCLO                    1.00000E-12   0.00000E+00   3.25360E-20   -19.4876
 H2O2                    1.00000E-12   0.00000E+00   3.68420E-21   -20.4337
 HCLO2                   1.00000E-12   0.00000E+00   1.28717E-37   -36.8904
 H2                      1.00000E-12   0.00000E+00   5.39110E-43   -42.2683
 HO2-1                   1.00000E-12   0.00000E+00   7.49315E-26   -25.1253
 CLO4-1                  1.00000E-12   0.00000E+00   8.09139E-33   -32.0920
 CLO3-1                  1.00000E-12   0.00000E+00   1.41605E-30   -29.8489
 CLO2-1                  1.00000E-12   0.00000E+00   1.29472E-32   -31.8878
 CLO2                    1.00000E-12   0.00000E+00   4.84011E-38   -37.3151
 CLO-1                   1.00000E-12   0.00000E+00   6.77886E-21   -20.1688
 CL2                     1.00000E-12   0.00000E+00   4.80004E-25   -24.3188
 Solution Properties:   pH =   6.9828    Eh =    0.7417 V     I =   0.0856
                        pe =  12.5375    Ah =   71.5647 kJ   m* =   0.1711
                        Aw =   0.9966    Os =    1.1033
                        At1= 1.0000E-12  At2= 1.2248E-07 (equiv_mol/kg_H2O)
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 AQUEOUS                 ENTERED    0.00000000E+00  5.56795440E+01
 SUSPENDED PHASES:
 REF_ELECTRODE NAOH_S2 NAOH NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O HCP_A3
 HALITE FCC_A1 BCC_A2 GAS
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.
 N=55.679543
 N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042542E-8,
    N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: @@... Calculating an initial equilibrium with all phases presented:
POLY_3: @@                                                  (except for REF_ELE)
POLY_3: c-st p *=ent 0
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY_3: @@ ..... Always setting the REF_ELECTRODE phase as SUSPENDED:
POLY_3: c-st p REF_ELE=sus
   ... the command in full is CHANGE_STATUS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 NAOH_S2                 ENTERED    0.00000000E+00  0.00000000E+00
 NAOH                    ENTERED    0.00000000E+00  0.00000000E+00
 NAO2                    ENTERED    0.00000000E+00  0.00000000E+00
 NA2O_S3                 ENTERED    0.00000000E+00  0.00000000E+00
 NA2O_S2                 ENTERED    0.00000000E+00  0.00000000E+00
 NA2O2_S2                ENTERED    0.00000000E+00  0.00000000E+00
 NA2O2                   ENTERED    0.00000000E+00  0.00000000E+00
 NA2O                    ENTERED    0.00000000E+00  0.00000000E+00
 HCP_A3                  ENTERED    0.00000000E+00  0.00000000E+00
 HALITE                  ENTERED    0.00000000E+00  0.00000000E+00
 FCC_A1                  ENTERED    0.00000000E+00  0.00000000E+00
 BCC_A2                  ENTERED    0.00000000E+00  0.00000000E+00
 AQUEOUS                 ENTERED    0.00000000E+00  5.58000000E+01
 GAS                     ENTERED    0.00000000E+00  0.00000000E+00
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated          749  grid points in            0  s
```

```
 Found the set of lowest grid points in            0  s
 Calculated POLY solution       1 s, total time     1  s
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
    N(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.56795E+01,  Mass in grams  1.00500E+03
 Total Gibbs energy -1.70630E+07,  Enthalpy -1.59010E+07,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                     5.5508E+01  9.9693E-01 9.9654E-01 -8.5871E+00 AQUEOUS
 H+1                    -9.7239E-08 -1.7464E-09 1.0405E-07 -3.9858E+04 SER
 ZE                      8.6043E-08  1.5453E-09 3.4476E+12  7.1565E+04 REF_ELEC
 NA                      8.5554E-02  1.5365E-03 4.5046E-63 -3.5588E+05 SER
 CL                      8.5554E-02  1.5365E-03 4.1623E-18 -9.9210E+04 SER

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00  Mole fractions:
 H2O  9.96927E-01  NA   1.53654E-03  H+1 -1.74641E-09
 CL   1.53654E-03  ZE   1.54532E-09
 Constitution:           SiteFraction    Molality      Activity      log10Act
 H2O                     9.96927E-01   5.55084E+01   9.96605E-01    -0.0015
 CL-1                    1.53654E-03   8.55538E-02   6.73425E-02    -1.1717
 NA+1                    1.53654E-03   8.55538E-02   6.73424E-02    -1.1717
 H+1                     2.37132E-09   1.32034E-07   1.04050E-07    -6.9828
 OH-1                    2.19965E-09   1.22476E-07   9.63757E-08    -7.0160
 O2                      4.70270E-10   2.61844E-08   2.61828E-08    -7.5820
 O3                      1.00000E-12   0.00000E+00   2.70935E-38   -37.5671
 HCLO                    1.00000E-12   0.00000E+00   3.25360E-20   -19.4876
 H2O2                    1.00000E-12   0.00000E+00   3.68420E-21   -20.4337
 HCLO2                   1.00000E-12   0.00000E+00   1.28717E-37   -36.8904
 H2                      1.00000E-12   0.00000E+00   5.39110E-43   -42.2683
 HO2-1                   1.00000E-12   0.00000E+00   7.49315E-26   -25.1253
 CLO4-1                  1.00000E-12   0.00000E+00   8.09139E-33   -32.0920
 CLO3-1                  1.00000E-12   0.00000E+00   1.41605E-30   -29.8489
 CLO2-1                  1.00000E-12   0.00000E+00   1.29472E-32   -31.8878
 CLO2                    1.00000E-12   0.00000E+00   4.84011E-38   -37.3151
 CLO-1                   1.00000E-12   0.00000E+00   6.77886E-21   -20.1688
 CL2                     1.00000E-12   0.00000E+00   4.80004E-25   -24.3188
 Solution Properties:   pH =   6.9828    Eh =    0.7417 V     I =   0.0856
                        pe =  12.5375    Ah =   71.5647 kJ   m* =   0.1711
                        Aw =   0.9966    Os =    1.1033
                        At1= 1.0000E-12  At2= 1.2248E-07 (equiv_mol/kg_H2O)
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 AQUEOUS                 ENTERED    0.00000000E+00  5.56795440E+01
 GAS                     ENTERED   -3.45348171E+00  0.00000000E+00
 HALITE                  ENTERED   -4.51928847E+00  0.00000000E+00
 NAOH                    ENTERED   -1.73748744E+01  0.00000000E+00
 BCC_A2                  ENTERED   -1.75296172E+01  0.00000000E+00
 FCC_A1                  ENTERED   -1.75296172E+01  0.00000000E+00
 NAOH_S2                 ENTERED   -1.79397738E+01  0.00000000E+00
 NAO2                    ENTERED   -1.99949604E+01  0.00000000E+00
 NA2O2                   ENTERED   -2.60508816E+01  0.00000000E+00
 NA2O2_S2                ENTERED   -2.64093970E+01  0.00000000E+00
 NA2O                    ENTERED   -4.24124745E+01  0.00000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.25799150E+01
 NA2O_S2 NA2O_S3 HCP_A3
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.
 N=55.679543
 N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042554E-8,
    N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
```

```
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@
POLY_3: @@ As shown here, 0.5wt% of Nacl (in 1 kg of H2O) is equivalent to
POLY_3: @@   0.085554 molality of NaCl.
POLY_3: @@
POLY_3:
POLY_3: @@... Saving the workspace for the H2O-NaCl system:
POLY_3: save TCEX53_a.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: @@ ======================================================================
POLY_3: @@ Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co) system
POLY_3: @@ **********************************************************************
POLY_3: @@   To demonstrate how to define the initial amount of alloy
POLY_3: @@       in an aqueous-bearing heterogeneous interaction system:
POLY_3: @@   ----------------------------------------------------------------
POLY_3: @@   Note: We are interested in only the BCC_A2 and FCC_A1 phases in
POLY_3: @@           the Fe-based alloy, in the current testing calculation.
POLY_3: @@         One may consider other possible phases (which exist in the
POLY_3: @@           applied steel material) if necessary.
POLY_3: @@
POLY_3: go d
   ... the command in full is GOTO_MODULE
TDB_PAQ2: rej sys
   ... the command in full is REJECT
 H                      O                      ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE               DIAMOND_A4             FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12               CUB_A13                CHI_A12
 FE4N                   FECN_CHI  REJECTED
 CEMENTITE              M23C6                  M7C3
 M5C2                   M3C2                   KSI_CARBIDE
 PI  REJECTED
 FE3C                   NI3C                   CR3C2
 CR7C3                  CR23C6  REJECTED
 COCO3                  FECO3                  NAHCO3
 NA2CO3                 NA2CO3_S2              NICO3
 CRC6O6  REJECTED
 CO3N                   CRN                    CR2N
 FE2N                   NI3N  REJECTED
 NANO2                  NANO2_S2               NANO3
   REJECTED
 COCL2                  CRCL2                  CRCL3
 FECL2                  FECL3                  NICL2
   REJECTED
 FECLO                  NACLO4                 NACLO4_S2
   REJECTED
 REINITIATING GES5 .....
TDB_PAQ2: sw SSOL4
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Alloy Solutions Database v4

 VA  DEFINED
 FCC_L102               FCC_L12  REJECTED
 ALNI_B2                A2_BCC                 BCC_B2
   REJECTED
 GAS:G  REJECTED
 IONIC_LIQUID:Y         BI2O3_LIQUID:Y         CORUNDUM:I
   REJECTED
TDB_SSOL4: d-sys Fe Cr Ni Co
   ... the command in full is DEFINE_SYSTEM
 FE                     CR                     NI
 CO  DEFINED
TDB_SSOL4: l-sys const
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :CO CR FE NI:
  > Metallic Liquid solution, also with Mg2Sn.
 FCC_A1      :CO CR FE NI:VA:
  > This is also the MC(1-x) carbide or nitride.
 BCC_A2      :CO CR FE NI:VA:
 HCP_A3      :CO CR FE NI:VA:
  > This is also the M2C carbide and M2N nitride.
```

```
 HCP_ZN      :CR:VA:
 TETRAGONAL_U :FE:
 CHI_A12     :CR FE:CR:CR FE:
 CBCC_A12    :CO CR FE NI:VA:
  > This is also the alpha-Mn phase.
 CUB_A13     :CO CR FE NI:VA:
  > This is also the beta-Mn phase.
 ORTHORHOMBIC_A20 :FE:
 SIGMA       :CO FE NI:CR:CO CR FE NI:
 HIGH_SIGMA  :FE:CR:CR FE:
 LAVES_C14   :CO CR FE NI:CO CR FE NI:
 LAVES_C15   :CO CR FE NI:CO CR FE NI:
 LAVES_C36   :CO CR NI:CO CR NI:
 FE4N        :CO FE NI:VA:
 AL5FE4      :FE:
 CONB_LAMBDA :CO:CO:
 CRSI2       :CR:CR:
 CR3SI_A15   :CR:CR:
 FESB        :FE:FE:
 FEU6        :FE:FE:
 FE2U        :FE:FE:
 FEUZR_DELTA :FE:FE:
 FEZR2       :FE:FE:
 FEZR3       :FE:FE:
 NI3NB       :NI:NI:
 NI3TI       :NI:NI:VA:
 NI3V        :NI:NI:
TDB_SSOL4: rej-ph *
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  HCP_ZN                  TETRAGONAL_U
 CHI_A12                 CBCC_A12                CUB_A13
 ORTHORHOMBIC_A20        SIGMA                   HIGH_SIGMA
 LAVES_C14               LAVES_C15               LAVES_C36
 FE4N                    AL5FE4                  CONB_LAMBDA
 CRSI2                   CR3SI_A15               FESB
 FEU6                    FE2U                    FEUZR_DELTA
 FEZR2                   FEZR3                   NI3NB
 NI3TI                   NI3V  REJECTED
TDB_SSOL4: rest-ph FCC_A1 BCC_A2
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2  RESTORED
TDB_SSOL4: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_SSOL4: @?<Hit_return_to_continue>
TDB_SSOL4:
TDB_SSOL4: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3:
POLY_3: @@... One can turn on the Global Minimization in the calculations:
POLY_3: @@ AD_OP E_C y,,,,,,,,,,,,
POLY_3:
POLY_3: s-c p=1e5 t=298.15
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@... The following conditions [system-size B and initial bulk
POLY_3: @@      composition w(i) of Fe-alloy] corresponds to the total
POLY_3: @@      initial amount of Fe-based alloy in the interaction,
POLY_3: @@      i.e., 1 gram of steel (Fe-10Cr-5Ni-1Co wt%).
POLY_3: s-c B=1  w(Cr)=.10 w(Ni)=.05 w(Co)=.01
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: l-c
```

```
   ... the command in full is LIST_CONDITIONS
 P=1E5, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
 Calculated         3638  grid points in            0  s
 Found the set of lowest grid points in             0  s
 Creating a new composition set BCC_A2#2
 Creating a new composition set BCC_A2#3
 Calculated POLY solution       0 s, total time     0  s
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL4

 Conditions:
 P=1E5, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.79859E-02,  Mass in grams  1.00000E+00
 Total Gibbs energy -1.58617E+02,  Enthalpy -1.09823E+01,  Volume  1.06647E-07

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 CO                      1.6968E-04  9.4343E-03 4.4119E-08 -4.1985E+04 SER
 CR                      1.9232E-03  1.0693E-01 5.8918E-02 -7.0195E+03 SER
 FE                      1.5041E-02  8.3627E-01 3.7073E-02 -8.1679E+03 SER
 NI                      8.5193E-04  4.7367E-02 7.7089E-04 -1.7769E+04 SER

 BCC_A2#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.4642E-02, Mass 8.1822E-01, Volume fraction 9.6230E-01  Mole fractions:
 FE  9.87119E-01  CO  1.15887E-02  NI  8.18003E-04  CR  4.74422E-04

 BCC_A2#3                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.9164E-03, Mass 9.9645E-02, Volume fraction 6.9591E-06  Mole fractions:
 CR  9.99945E-01  FE  5.45402E-05  CO  1.93503E-11  NI  8.91029E-12

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.4280E-03, Mass 8.2138E-02, Volume fraction 3.7694E-02  Mole fractions:
 NI  5.88203E-01  FE  4.11792E-01  CO  5.30486E-06  CR  6.99036E-09
POLY_3: l-st cp
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 CO                      ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 NI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FCC_A1                  ENTERED    0.00000000E+00  1.42800647E-03
 BCC_A2#3                ENTERED    0.00000000E+00  1.91638306E-03
 BCC_A2#1                ENTERED    0.00000000E+00  1.46415479E-02
 SUSPENDED PHASES:
 BCC_A2#2
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1
 N=1.7985937E-2
 N(CO)=1.6968422E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY_3: @?<Hit_return_to_continue>
POLY_3: @@
POLY_3: @@ As shown here, 1 gram of steel (Fe-10Cr-5Ni-1Co wt%)
POLY_3: @@   is equivalent to:
POLY_3: @@       n(Fe) = 1.5041094E-2
POLY_3: @@       n(Cr) = 1.9232249E-3
POLY_3: @@       n(Ni) = 8.5193389E-4
POLY_3: @@       n(Co) = 1.6968422E-4
POLY_3: @@
POLY_3:
POLY_3: @@... Saving the workspace for the Fe-Cr-Ni-Co system:
POLY_3: save TCEX53_b.POLY3 y
   ... the command in full is SAVE_WORKSPACES
```

```
POLY_3:
POLY_3: @@ ======================================================================
POLY_3: @@ Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl system
POLY_3: @@ **********************************************************************
POLY_3: @@   Bulk composition in the heterogeneous interaction system:
POLY_3: @@          b(H2O)  = 1000
POLY_3: @@          n(NaCl) = 0.085554
POLY_3: @@          n(Fe) = 1.5041094E-2
POLY_3: @@          n(Cr) = 1.9232249E-3
POLY_3: @@          n(Ni) = 8.5193389E-4
POLY_3: @@          n(Co) = 1.6968422E-4
POLY_3:
POLY_3: @@... Retrieving data from the PAQ2 or PAQS2 database:
POLY_3: go d
   ... the command in full is GOTO_MODULE
TDB_SSOL4: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 FCC_L102               FCC_L12  REJECTED
 ALNI_B2                A2_BCC                 BCC_B2
   REJECTED
 GAS:G  REJECTED
 IONIC_LIQUID:Y         BI2O3_LIQUID:Y         CORUNDUM:I
   REJECTED
 REINITIATING GES5 .....
TDB_SSOL4: @@ ------ switch on PAQ2 or PAQS2
TDB_SSOL4: sw PAQ2
   ... the command in full is SWITCH_DATABASE
 Current database: TCS Public Aqueous Soln (SIT) TDB v2

 H                      O                      ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE               DIAMOND_A4             FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12               CUB_A13                CHI_A12
 FE4N                   FECN_CHI  REJECTED
 CEMENTITE              M23C6                  M7C3
 M5C2                   M3C2                   KSI_CARBIDE
 PI  REJECTED
 FE3C                   NI3C                   CR3C2
 CR7C3                  CR23C6  REJECTED
 COCO3                  FECO3                  NAHCO3
 NA2CO3                 NA2CO3_S2              NICO3
 CRC6O6  REJECTED
 CO3N                   CRN                    CR2N
 FE2N                   NI3N  REJECTED
 NANO2                  NANO2_S2               NANO3
   REJECTED
 COCL2                  CRCL2                  CRCL3
 FECL2                  FECL3                  NICL2
   REJECTED
 FECLO                  NACLO4                 NACLO4_S2
   REJECTED
TDB_PAQ2: d-sys H O Na Cl Fe Cr Ni Co
   ... the command in full is DEFINE_SYSTEM
 NA                     CL                     FE
 CR                     NI                     CO
   DEFINED
TDB_PAQ2: l-sys const
   ... the command in full is LIST_SYSTEM
 AQUEOUS:A   :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CL2 CL-1 CLO2 CLO-1 CLO2-1
  CLO3-1 CLO4-1 HCLO HCLO2 CO+2 CO+3 CR+2 CR+3 CROH+2 CRO+1 CRO2-1 HCRO2
  HCRO4-1 CRO4-2 CR2O7-2 FE+2 FE+3 FEOH+1 FEOH+2 FEO3H3-1 FE2O2H2+4 FECL+2
  NA+1 NI+2 NIOH+1:
  > Aqueous Solution: using the SIT Model (from TCAQ2 database)
 REF_ELECTRODE :ZE:
  > Reference Electrode for ZE potentail; always SUSPENDED in POLY.
 GAS:G       :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1CO1 CL1CR1 CL1CR1O1
  CL1CR1O2 CL1FE1 CL1NA1 CL1NI1 CL2CO1 CL2CR1 CL2CR1O1 CL2CR1O2 CL2FE1
  CL2NA2 CL2NI1 CL3CO1 CL3CR1 CL3CR1O1 CL3FE1 CL3NA3 CL4CO2 CL4CR1 CL4CR1O1
  CL4FE2 CL5CR1 CL6CR1 CL6FE2 CO CO1H1 CO1H2O2 CO1O1 CR CR1H1 CR1H1O1
  CR1H1O2 CR1H1O3 CR1H2O2 CR1H2O3 CR1H2O4 CR1H3O3 CR1H3O4 CR1H4O4 CR1H4O5
  CR1O1 CR1O2 CR1O3 CR2 CR2O1 CR2O2 CR2O3 FE FE1H1O1 FE1H1O2 FE1H2O2 FE1O1
```

```
 FE1O2 H H1NA1 H1NA1O1 H1NI1 H1NI1O1 H1O1 H1O2 H2 H2NA2O2 H2NI1O2 H2O1 H2O2
 NA NA1O1 NA2 NA2O1 NA2O2 NI NI1O1 O O2 O3:
 > Gaseous Mixture, using the ideal gas model
FCC_A1      :CO CR FE NA NI O:VA:
 > This is also the MX (X=C,N) solution phase.
BCC_A2      :CO CR FE NA NI O:VA:
 > This is also the MX3 (X=C,N) solution phase.
HCP_A3      :CO CR FE NA NI:VA:
 > This is also the M2X (X=C,N) solution phase.
SIGMA       :CO FE NI:CR:CO CR FE NI:
HALITE      :NA1CL1:
WUSTITE     :FE0.947O1:
MAGNETITE   :FE3O4:
HEMATITE    :FE2O3:
FE2O3_GAMMA :FE2O3:
FEO2H2      :FE1H2O2:
FEO3H3      :FE1H3O3:
FEOOH       :FE1H1O2:
FE2O2O2H2   :FE2H2O4:
COO         :CO1O1:
CO3O4       :CO3O4:
COO2H2      :CO1H2O2:
CRO2        :CR1O2:
CRO3        :CR1O3:
CR2O3       :CR2O3:
CR5O12      :CR5O12:
CR8O21      :CR8O21:
NAO2        :NA1O2:
NA2O        :NA2O1:
NA2O_S2     :NA2O1:
NA2O_S3     :NA2O1:
NA2O2       :NA2O2:
NA2O2_S2    :NA2O2:
NAOH        :H1NA1O1:
NAOH_S2     :H1NA1O1:
NIO         :NI1O1:
NIO_S2      :NI1O1:
NIO2H2      :H2NI1O2:
NIOOH       :H1NI1O2:
FECR2O4     :CR2FE1O4:
COCR2O4     :CO1CR2O4:
NICR2O4     :CR2NI1O4:
NA2CR2O4    :CR2NA2O4:
COFE2O4     :CO1FE2O4:
NIFE2O4     :FE2NI1O4:
NA2CRO4     :CR1NA2O4:
NA2CRO4_S2  :CR1NA2O4:
NA2FEO2     :FE1NA1O2:
TDB_PAQ2: @?<Hit_return_to_continue>
TDB_PAQ2:
TDB_PAQ2: rej ph  HCP_A3 CBCC_A12 CUB_A13 CHI_A12 Fe4N
   ... the command in full is REJECT
 HCP_A3  REJECTED
TDB_PAQ2: rej ph  SIGMA
   ... the command in full is REJECT
 SIGMA  REJECTED
TDB_PAQ2: rej ph  NaH
   ... the command in full is REJECT
TDB_PAQ2: get
   ... the command in full is GET_DATA
 REINITIATING GES5 .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data
```

```
  'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
      -Cl system.'
  'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
      -Cr-Na-Ni-C-H-O-N-S-Cl system.'
  'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
      -Na-Ni-C-H-O-N-S-Cl system.'
  'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
      only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
      from TCAQ2 which covers totally 83 elements and contains many more
      aqueous solution species.'
 -OK-
TDB_PAQ2: @?<Hit_return_to_continue>
TDB_PAQ2:
TDB_PAQ2: @@... Defining system-components and their proper reference states:
TDB_PAQ2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32,  Dec 2007
POLY_3: d-com H2O H+1 ZE Na Cl Fe Cr Ni Co
   ... the command in full is DEFINE_COMPONENTS
POLY_3: s-r-s H2O AQUEOUS * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s Ze  REF_ELE * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY_3: l-st c
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT              STATUS    REF. STATE     T(K)           P(Pa)
 VA                     ENTERED   SER
 H2O                    ENTERED   AQUEOUS        *              100000
 H+1                    ENTERED   SER
 ZE                     ENTERED   REF_ELECTRODE  *              100000
 NA                     ENTERED   SER
 CL                     ENTERED   SER
 FE                     ENTERED   SER
 CR                     ENTERED   SER
 NI                     ENTERED   SER
 CO                     ENTERED   SER
POLY_3:
POLY_3: @@... Defining some symbols (constants/variables/functions/tables):
POLY_3: @@    ************************************************************
POLY_3: @@  One may choose to just define some important ones as shown here,
POLY_3: @@           e.g., RNF; pH, Eh
POLY_3: @@  ------------------------------------------------------------------
POLY_3: @@  Important: There are two ways of defining pH in aqueous system:
POLY_3: @@     A) Using the TDB-default reference state for H+1:
POLY_3: @@           pH = -log10[acr(H+1)]
POLY_3: @@              = -ln[acr(H+1)]*2.302585093
POLY_3: @@     B) Using the H+1(aqs) in AQUEOUS Phase as H+1 reference state:
POLY_3: @@           pH = -log10[activity(H+1,aqs)]          (traditional)
POLY_3: @@              = -log10[acr(H+1,AQUEOUS)*AH2O]
POLY_3: @@              = -ln[acr(H+1,AQUEOUS)*AH2O]*2.302585093
POLY_3: @@     Both definitions are entirely equivalent, and they always have
POLY_3: @@     the same pH value for the same condition for a defined system.
POLY_3: @@     Thermo-Calc GES/POLY/POURBAIX modules use the first one A).
POLY_3: @@
POLY_3: @@  ------------------------------------------------------------------
POLY_3: @@  Notes:
POLY_3: @@    If desired, one may also choose to define many other possible
POLY_3: @@      symbols (for the convenience of plotting) on the same scope
POLY_3: @@      of the POURBAIX-Module.
POLY_3: @@    A complete list of valid symbols for the Fe-Cr-Ni-Co-H2O-NaCl
POLY_3: @@      heterogeneous interaction system on the scope same as the
POLY_3: @@      automatically-defined symbols in the POURBAIX-Module can be
POLY_3: @@      found at the end of this MACRO file (only as a reference!).
POLY_3: @@  ------------------------------------------------------------------
POLY_3: @@
POLY_3: ent-sym const AH2O=55.508435
   ... the command in full is ENTER_SYMBOL
POLY_3: ent-sym const RNF =96485.309
   ... the command in full is ENTER_SYMBOL
POLY_3: ent-sym funct Eh = mur(ZE)/RNF;
   ... the command in full is ENTER_SYMBOL
```

```
POLY_3: ent-sym funct pH = -log10(acr(H+1));
   ... the command in full is ENTER_SYMBOL
POLY_3: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED CONSTANTS
    AH2O=55.508435, RNF=96485.309
 DEFINED FUNCTIONS AND VARIABLES%
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1) )
POLY_3:
POLY_3: @@... Defining the equilibrium conditions:
POLY_3: @@    ------------------------------------------------------------
POLY_3: @@     Defining P-T and bulk composition in the interaction system
POLY_3: @@     for calculating starting point [at e.g pH=7 & Eh=0 (V)]:
POLY_3: @@
POLY_3:
POLY_3: @@ ------ P-T conditions:
POLY_3: s-c p=1e5 t=298.15
   ... the command in full is SET_CONDITION
POLY_3: @@
POLY_3: @@      ... Alternatively, it can be manually input as below:
POLY_3: @@   s-c p=
POLY_3: @@ @?Pressure_in_Pascal:
POLY_3: @@   s-c t=
POLY_3: @@ @?Temperature_In_Kelvin:
POLY_3:
POLY_3: @@ ------ For Aqueous-involving interaction system, it is always
POLY_3: @@        recommended to define 1 kg of H2O, so that it is very
POLY_3: @@        convenient to consider molality quantities and other
POLY_3: @@        properties in aqueous solution.
POLY_3: s-c b(H2O)=1000
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ------ The following is equivalent to 0.085554 mole of NaCl
POLY_3: @@                                          in 1 kg of H2O:
POLY_3: s-c n(Na)=0.085554  n(Cl)=0.085554
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ------ For calculating Pourbaix diagrams or other diagrams in
POLY_3: @@        aqueous-involving interaction system, it is important
POLY_3: @@        to consider the so-called "effective interaction rate".
POLY_3: @@
POLY_3: @@     The following is equivalent to 1 gram of specified steel
POLY_3: @@        (Fe-10Cr-5Ni-1Co wt%) in an effective interaction with
POLY_3: @@        1 kg of H2O (dissolving 0.085554 mole of NaCl):
POLY_3: s-c n(Fe)=1.5041094E-2  n(Cr)=1.9232249E-3
   ... the command in full is SET_CONDITION
POLY_3: s-c n(Ni)=8.5193389E-4  n(Co)=1.6968422E-4
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ------ Let's calculate initial equilibrium at pH=7 & Eh=0 (V):
POLY_3: s-c lnacr(H+1)=-16.11809565  mur(Ze)=0
   ... the command in full is SET_CONDITION
POLY_3:
POLY_3: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
    LNACR(H+1)=-16.1181, MUR(ZE)=0
 DEGREES OF FREEDOM 0
POLY_3:
POLY_3: @@... One may turn off the Global Minimization in the calculations:
POLY_3: @@ AD_OP E_C n y 5000 y y 0 y 3 n ,,
POLY_3:
POLY_3: @@... Setting numerical limits:
POLY_3: @@  ------------------------------------------------------------
POLY_3: @@  Notes:
POLY_3: @@    For equilibrium calculations (single-point, stepping or mapping)
POLY_3: @@      of complex aqueous-bearing heterogeneous interaction systems,
POLY_3: @@      it is recommended to properly modify the numerical limits.
POLY_3: @@    The following command (changing the numerical limits from the
POLY_3: @@      default values "500 1E-6 1E-12 N" to "2000 1E-4 1E-12 N")
POLY_3: @@      will bring two changes:
POLY_3: @@      1) The change on "Maximum number of iterations" from the
```

```
POLY_3: @@           default value 500 to 2000, which enforces 4 times more
POLY_3: @@           iterations for each of the calculations in order to
POLY_3: @@           obtain stable equilibria;
POLY_3: @@      2) The change on "Required accuracy" from the default value
POLY_3: @@           1E-6 to 1E-4, which allows less accurate calculations
POLY_3: @@           and it is thus easier/faster to converge.
POLY_3: @@      The "Smallest fraction" remains 1E-12 (site fraction), and
POLY_3: @@      the "Approximate driving force for metastable phases" keeps
POLY_3: @@      the default value of "N" (meaning it should always precisely
POLY_3: @@      calculate driving forces for metastable phases).
POLY_3: @@    Such changes in the numerical limits are essential and useful
POLY_3: @@      for making sure of finding a converged solution of stable
POLY_3: @@      equilbria, especially when the heterogeneous interaction
POLY_3: @@      system becomes more and more complicated.
POLY_3: @@  ----------------------------------------------------------------
POLY_3: @@
POLY_3: s-n-l 2000 1e-4 1e-12 n
   ... the command in full is SET_NUMERICAL_LIMITS
 LIMITATIONS of the present version of Thermo-Calc
 Max number of elements                      :  40
 Max number of species                       :1000
 Max number of sublattices in a phase        :  10
 Max number of constituents in a phase:      : 200
 Max number of constituents in an ideal phase :1000

POLY_3:
POLY_3: @@... Calculating an initial equilibrium with only AQUEOUS presented:
POLY_3: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 AQUEOUS                ENTERED    0.00000000E+00  5.97059994E+03
 SUSPENDED PHASES:
 WUSTITE REF_ELECTRODE NIO_S2 NIOOH NIO2H2 NIO NIFE2O4 NICR2O4 NAOH_S2 NAOH
 NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O NA2FEO2 NA2CRO4_S2 NA2CRO4 NA2CR2O4
 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4 FE2O3_GAMMA FE2O2O2H2
 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO2H2 COO COFE2O4 COCR2O4 CO3O4 BCC_A2
 GAS
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated           5  grid points in           0  s
    86 ITS,  CPU TIME USED   1 SECONDS
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
    LNACR(H+1)=-16.1181, MUR(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.57254E+01,  Mass in grams  1.00599E+03
 Total Gibbs energy -1.70641E+07,  Enthalpy -1.59024E+07,  Volume -4.21627E-08

 Component              Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                    5.5508E+01  9.9611E-01 9.9606E-01 -9.7846E+00 AQUEOUS
 H+1                   -1.0027E-02 -1.7993E-04 1.0000E-07 -3.9956E+04 SER
 ZE                     3.7895E-02  6.8003E-04 1.0000E+00  3.8918E-13 REF_ELEC
 NA                     8.5554E-02  1.5353E-03 1.5211E-50 -2.8436E+05 SER
 CL                     8.5554E-02  1.5353E-03 1.1822E-30 -1.7083E+05 SER
 FE                     1.5041E-02  2.6991E-04 1.2285E-18 -1.0223E+05 SER
 CR                     1.9232E-03  3.4513E-05 1.6596E-45 -2.5561E+05 SER
 NI                     8.5193E-04  1.5288E-05 6.0058E-14 -7.5468E+04 SER
 CO                     1.6969E-04  3.0451E-06 3.2709E-16 -8.8391E+04 SER

 AQUEOUS                    Status ENTERED     Driving force  0.0000E+00
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 Moles 5.5725E+01, Mass 1.0060E+03, Volume fraction 1.0000E+00  Mole fractions:
 H2O  9.96107E-01  ZE   6.80033E-04  NI   1.52881E-05
 CL   1.53528E-03  FE   2.69915E-04  CO   3.04507E-06
 NA   1.53528E-03  CR   3.45128E-05  H+1 -1.79930E-04
 Constitution:           SiteFraction    Molality      Activity      log10Act
 H2O                     9.96604E-01   5.55084E+01   9.96157E-01    -0.0017
 CL-1                    1.53628E-03   8.55669E-02   6.59412E-02    -1.1808
 NA+1                    1.53628E-03   8.55668E-02   6.59591E-02    -1.1807
 FE+2                    1.56791E-04   8.73285E-03   3.08752E-03    -2.5104
 FEOH+1                  1.13299E-04   6.31050E-03   4.86919E-03    -2.3125
 CRO+1                   3.00742E-05   1.67506E-03   1.29248E-03    -2.8886
 NI+2                    1.52852E-05   8.51348E-04   3.02381E-04    -3.5194
 CROH+2                  3.38459E-06   1.88513E-04   6.68404E-05    -4.1750
 CO+2                    3.04704E-06   1.69713E-04   6.02723E-05    -4.2199
 HCRO2                   1.05904E-06   5.89860E-05   5.89804E-05    -4.2293
 NIOH+1                  1.28111E-08   7.13548E-07   5.50574E-07    -6.2592
 CR+3                    1.12056E-08   6.24127E-07   6.07389E-08    -7.2165
 CRO2-1                  6.16636E-09   3.43451E-07   2.65007E-07    -6.5767
 OH-1                    2.33522E-09   1.30066E-07   1.00231E-07    -6.9990
 H+1                     2.32641E-09   1.29576E-07   1.00000E-07    -7.0000
 FEOH+2                  1.10316E-12   6.14435E-11   2.17858E-11   -10.6618
 O3                      1.00000E-12   0.00000E+00   2.0444E-113  -112.6894
 H2                      1.00000E-12   0.00000E+00   5.91876E-18   -17.2278
 FEO3H3-1                1.00000E-12   0.00000E+00   4.15261E-44   -43.3817
 FECL+2                  1.00000E-12   0.00000E+00   6.77824E-16   -15.1689
 FE2O2H2+4               1.00000E-12   0.00000E+00   2.05117E-20   -19.6880
 FE+3                    1.00000E-12   0.00000E+00   3.61605E-16   -15.4418
 H2O2                    1.00000E-12   0.00000E+00   3.35251E-46   -45.4746
 HCLO                    1.00000E-12   0.00000E+00   2.78757E-45   -44.5548
 CRO4-2                  1.00000E-12   0.00000E+00   1.67198E-26   -25.7768
 HCLO2                   1.00000E-12   0.00000E+00   1.00400E-87   -86.9983
 HCRO4-1                 1.00000E-12   0.00000E+00   5.05296E-27   -26.2965
 CR2O7-2                 1.00000E-12   0.00000E+00   9.28132E-52   -51.0324
 HO2-1                   1.00000E-12   0.00000E+00   7.09471E-51   -50.1491
 CR+2                    1.00000E-12   0.00000E+00   2.91278E-15   -14.5357
 CO+3                    1.00000E-12   0.00000E+00   7.96286E-38   -37.0989
 O2                      1.00000E-12   0.00000E+00   2.17014E-58   -57.6635
 CLO4-1                  1.00000E-12   0.00000E+00   5.4430E-133  -132.2642
 CLO3-1                  1.00000E-12   0.00000E+00   1.0463E-105  -104.9803
 CLO2-1                  1.00000E-12   0.00000E+00   1.05079E-82   -81.9785
 CLO2                    1.00000E-12   0.00000E+00   1.1394E-100   -99.9433
 CLO-1                   1.00000E-12   0.00000E+00   6.04312E-46   -45.2187
 CL2                     1.00000E-12   0.00000E+00   3.87205E-50   -49.4121
 Solution Properties:   pH =   7.0000    Eh =    0.0000 V     I =   0.1094
                        pe =   0.0000    Ah =    0.0000 kJ   m* =   0.1891
                        Aw =   0.9962    Os =    1.1300
                        At1= 1.0000E-12  At2= 1.3007E-07 (equiv_mol/kg_H2O)
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 AQUEOUS                 ENTERED    0.00000000E+00  5.57253960E+01
 SUSPENDED PHASES:
 WUSTITE REF_ELECTRODE NIO_S2 NIOOH NIO2H2 NIO NIFE2O4 NICR2O4 NAOH_S2 NAOH
 NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O NA2FEO2 NA2CRO4_S2 NA2CRO4 NA2CR2O4
 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4 FE2O3_GAMMA FE2O2O2H2
 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO2H2 COO COFE2O4 COCR2O4 CO3O4 BCC_A2
 GAS
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.9899
 N=55.725398
 N(H2O)=55.508435, N(H+1)=-1.0026681E-2, N(ZE)=3.789509E-2, N(NA)=8.5554E-2,
    N(CL)=8.5554078E-2, N(FE)=1.5041101E-2, N(CR)=1.9232397E-3,
    N(NI)=8.5193389E-4, N(CO)=1.6968753E-4
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: @@... Calculating an initial equilibrium with all phases presented:
POLY_3: @@                                                  (except for REF_ELE)
POLY_3: c-st p *=ent 0
   ... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY_3: @@ ...... Always setting the REF_ELECTRODE phase as SUSPENDED:
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POLY_3: c-st p REF_ELE=sus
   ... the command in full is CHANGE_STATUS
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 WUSTITE                 ENTERED    0.00000000E+00  0.00000000E+00
 NIO_S2                  ENTERED    0.00000000E+00  0.00000000E+00
 NIOOH                   ENTERED    0.00000000E+00  0.00000000E+00
 NIO2H2                  ENTERED    0.00000000E+00  0.00000000E+00
 NIO                     ENTERED    0.00000000E+00  0.00000000E+00
 NIFE2O4                 ENTERED    0.00000000E+00  0.00000000E+00
 NICR2O4                 ENTERED    0.00000000E+00  0.00000000E+00
 NAOH_S2                 ENTERED    0.00000000E+00  0.00000000E+00
 NAOH                    ENTERED    0.00000000E+00  0.00000000E+00
 NAO2                    ENTERED    0.00000000E+00  0.00000000E+00
 NA2O_S3                 ENTERED    0.00000000E+00  0.00000000E+00
 NA2O_S2                 ENTERED    0.00000000E+00  0.00000000E+00
 NA2O2_S2                ENTERED    0.00000000E+00  0.00000000E+00
 NA2O2                   ENTERED    0.00000000E+00  0.00000000E+00
 NA2O                    ENTERED    0.00000000E+00  0.00000000E+00
 NA2FEO2                 ENTERED    0.00000000E+00  0.00000000E+00
 NA2CRO4_S2              ENTERED    0.00000000E+00  0.00000000E+00
 NA2CRO4                 ENTERED    0.00000000E+00  0.00000000E+00
 NA2CR2O4                ENTERED    0.00000000E+00  0.00000000E+00
 MAGNETITE               ENTERED    0.00000000E+00  0.00000000E+00
 HEMATITE                ENTERED    0.00000000E+00  0.00000000E+00
 HALITE                  ENTERED    0.00000000E+00  0.00000000E+00
 FEOOH                   ENTERED    0.00000000E+00  0.00000000E+00
 FEO3H3                  ENTERED    0.00000000E+00  0.00000000E+00
 FEO2H2                  ENTERED    0.00000000E+00  0.00000000E+00
 FECR2O4                 ENTERED    0.00000000E+00  0.00000000E+00
 FE2O3_GAMMA             ENTERED    0.00000000E+00  0.00000000E+00
 FE2O2O2H2               ENTERED    0.00000000E+00  0.00000000E+00
 FCC_A1                  ENTERED    0.00000000E+00  0.00000000E+00
 CRO3                    ENTERED    0.00000000E+00  0.00000000E+00
 CRO2                    ENTERED    0.00000000E+00  0.00000000E+00
 CR8O21                  ENTERED    0.00000000E+00  0.00000000E+00
 CR5O12                  ENTERED    0.00000000E+00  0.00000000E+00
 CR2O3                   ENTERED    0.00000000E+00  0.00000000E+00
 COO2H2                  ENTERED    0.00000000E+00  0.00000000E+00
 COO                     ENTERED    0.00000000E+00  0.00000000E+00
 COFE2O4                 ENTERED    0.00000000E+00  0.00000000E+00
 COCR2O4                 ENTERED    0.00000000E+00  0.00000000E+00
 CO3O4                   ENTERED    0.00000000E+00  0.00000000E+00
 BCC_A2                  ENTERED    0.00000000E+00  0.00000000E+00
 AQUEOUS                 ENTERED    0.00000000E+00  5.58362320E+01
 GAS                     ENTERED    0.00000000E+00  0.00000000E+00
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY_3: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Calculated         2941  grid points in            0  s
   483 ITS,  CPU TIME USED   2 SECONDS
POLY_3: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
    LNACR(H+1)=-16.1181, MUR(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.56976E+01,  Mass in grams  1.00595E+03
 Total Gibbs energy -1.70627E+07,  Enthalpy -1.59010E+07,  Volume -6.20719E-15

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                     5.5508E+01  9.9660E-01 9.9654E-01 -8.5924E+00 AQUEOUS
 H+1                    -5.2910E-02 -9.4995E-04 1.0000E-07 -3.9956E+04 SER
 ZE                      5.2936E-02  9.5042E-04 1.0000E+00 -4.0144E-12 REF_ELEC
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NA                     8.5554E-02  1.5360E-03 1.5537E-50 -2.8431E+05 SER
CL                     8.5554E-02  1.5360E-03 1.2078E-30 -1.7077E+05 SER
FE                     1.5041E-02  2.7005E-04 5.2232E-26 -1.4431E+05 SER
CR                     1.9232E-03  3.4530E-05 1.2572E-53 -3.0196E+05 SER
NI                     8.5193E-04  1.5296E-05 1.0073E-15 -8.5603E+04 SER
CO                     1.6969E-04  3.0466E-06 1.5331E-20 -1.1310E+05 SER

AQUEOUS                    Status ENTERED     Driving force  0.0000E+00
Moles 5.5653E+01, Mass 1.0045E+03, Volume fraction 1.0000E+00  Mole fractions:
H2O  9.96925E-01  ZE   4.71298E-07  FE   1.68577E-11
CL   1.53727E-03  NI   2.36160E-07  CR   1.00000E-11
NA   1.53727E-03  CO   1.32447E-10  H+1 -3.11048E-10
Constitution:          SiteFraction    Molality      Activity      log10Act
H2O                    9.96925E-01   5.55084E+01   9.96603E-01    -0.0015
CL-1                   1.53727E-03   8.55949E-02   6.73704E-02    -1.1715
NA+1                   1.53727E-03   8.55948E-02   6.73703E-02    -1.1715
NI+2                   2.35950E-07   1.31376E-05   5.07139E-06    -5.2949
OH-1                   2.28889E-09   1.27444E-07   1.00279E-07    -6.9988
H+1                    2.27916E-09   1.26903E-07   1.00000E-07    -7.0000
NIOH+1                 2.10599E-10   1.17261E-08   9.23842E-09    -8.0344
CO+2                   1.31447E-10   7.31890E-09   2.82496E-09    -8.5490
FE+2                   6.13590E-12   3.41645E-10   1.31278E-10    -9.8818
FEOH+1                 4.72178E-12   2.62907E-10   2.07132E-10    -9.6838
O3                     1.00000E-12   0.00000E+00   2.0474E-113  -112.6888
HCLO                   1.00000E-12   0.00000E+00   2.84935E-45   -44.5453
H2O2                   1.00000E-12   0.00000E+00   3.35574E-46   -45.4742
HCLO2                  1.00000E-12   0.00000E+00   1.02675E-87   -86.9885
H2                     1.00000E-12   0.00000E+00   5.91876E-18   -17.2278
HCRO2                  1.00000E-12   0.00000E+00   4.47228E-13   -12.3495
FEOH+2                 1.00000E-12   0.00000E+00   9.26752E-19   -18.0330
HCRO4-1                1.00000E-12   0.00000E+00   3.83517E-35   -34.4162
FEO3H3-1               1.00000E-12   0.00000E+00   1.76819E-51   -50.7525
FECL+2                 1.00000E-12   0.00000E+00   2.94449E-23   -22.5310
FE2O2H2+4              1.00000E-12   0.00000E+00   3.71178E-35   -34.4304
FE+3                   1.00000E-12   0.00000E+00   1.53750E-23   -22.8132
HO2-1                  1.00000E-12   0.00000E+00   7.10153E-51   -50.1486
CROH+2                 1.00000E-12   0.00000E+00   5.06585E-13   -12.2953
CRO4-2                 1.00000E-12   0.00000E+00   1.26903E-34   -33.8965
CRO2-1                 1.00000E-12   0.00000E+00   2.00946E-15   -14.6969
CRO+1                  1.00000E-12   0.00000E+00   9.79571E-12   -11.0090
CR2O7-2                1.00000E-12   0.00000E+00   5.34416E-68   -67.2721
CR+3                   1.00000E-12   0.00000E+00   4.60120E-16   -15.3371
CR+2                   1.00000E-12   0.00000E+00   2.20654E-23   -22.6563
CO+3                   1.00000E-12   0.00000E+00   3.73219E-42   -41.4280
O2                     1.00000E-12   0.00000E+00   2.17223E-58   -57.6631
CLO4-1                 1.00000E-12   0.00000E+00   5.5717E-133  -132.2540
CLO3-1                 1.00000E-12   0.00000E+00   1.0705E-105  -104.9704
CLO2-1                 1.00000E-12   0.00000E+00   1.07460E-82   -81.9688
CLO2                   1.00000E-12   0.00000E+00   1.1652E-100   -99.9336
CLO-1                  1.00000E-12   0.00000E+00   6.17706E-46   -45.2092
CL2                    1.00000E-12   0.00000E+00   4.04171E-50   -49.3934
Solution Properties:   pH =   7.0000    Eh =    0.0000 V     I =   0.0856
                       pe =   0.0000    Ah =    0.0000 kJ   m* =   0.1712
                       Aw =   0.9966    Os =    1.1033
                       At1= 1.0000E-12  At2= 1.2745E-07 (equiv_mol/kg_H2O)

HEMATITE                   Status ENTERED     Driving force  0.0000E+00
Moles 3.3409E-02, Mass 1.0670E+00, Volume fraction 0.0000E+00  Mole fractions:
ZE   1.20000E+00  NI   0.00000E+00  NA   0.00000E+00
H2O  6.00000E-01  CR   0.00000E+00  CO   0.00000E+00
FE   4.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00

NIFE2O4                    Status ENTERED     Driving force  0.0000E+00
Moles 5.8715E-03, Mass 1.9660E-01, Volume fraction 0.0000E+00  Mole fractions:
ZE   1.14286E+00  NI   1.42857E-01  NA   0.00000E+00
H2O  5.71429E-01  CR   0.00000E+00  CO   0.00000E+00
FE   2.85714E-01  CL   0.00000E+00  H+1 -1.14286E+00

CR2O3                      Status ENTERED     Driving force  0.0000E+00
Moles 3.9597E-03, Mass 1.2037E-01, Volume fraction 0.0000E+00  Mole fractions:
ZE   1.20000E+00  NI   0.00000E+00  NA   0.00000E+00
H2O  6.00000E-01  FE   0.00000E+00  CO   0.00000E+00
CR   4.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00
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 COCR2O4                     Status ENTERED     Driving force  0.0000E+00
 Moles 1.1878E-03, Mass 3.8504E-02, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.14286E+00  CO   1.42857E-01  NA   0.00000E+00
 H2O  5.71429E-01  NI   0.00000E+00  FE   0.00000E+00
 CR   2.85714E-01  CL   0.00000E+00  H+1 -1.14286E+00
POLY_3: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 NIFE2O4                 ENTERED    0.00000000E+00  5.87153564E-03
 HEMATITE                ENTERED    0.00000000E+00  3.34088164E-02
 CR2O3                   ENTERED    0.00000000E+00  3.95971655E-03
 COCR2O4                 ENTERED    0.00000000E+00  1.18776501E-03
 AQUEOUS                 ENTERED    0.00000000E+00  5.56531280E+01
 FECR2O4                 ENTERED   -1.00759971E-01  0.00000000E+00
 FE2O2O2H2               ENTERED   -1.87297778E-01  0.00000000E+00
 FEOOH                   ENTERED   -2.26040225E-01  0.00000000E+00
 COFE2O4                 ENTERED   -8.14919243E-01  0.00000000E+00
 FEO3H3                  ENTERED   -1.15750993E+00  0.00000000E+00
 NICR2O4                 ENTERED   -1.41536242E+00  0.00000000E+00
 FE2O3_GAMMA             ENTERED   -1.46143265E+00  0.00000000E+00
 MAGNETITE               ENTERED   -1.55630225E+00  0.00000000E+00
 NIO2H2                  ENTERED   -3.14632974E+00  0.00000000E+00
 GAS                     ENTERED   -3.45624187E+00  0.00000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.15999889E+00
 NIO NIO_S2 HALITE COO2H2 FEO2H2 NA2CR2O4 NA2FEO2 CO3O4 WUSTITE COO CRO2
 NA2CRO4 NA2CRO4_S2 NIOOH CR5O12 NAOH NAOH_S2 CR8O21 CRO3 FCC_A1 BCC_A2 NA2O2
 NA2O2_S2 NA2O NA2O_S2 NA2O_S3 NAO2
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY_3: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.9467
 N=55.697556
 N(H2O)=55.508435, N(H+1)=-5.2910029E-2, N(ZE)=5.293624E-2, N(NA)=8.5554E-2,
    N(CL)=8.5554078E-2, N(FE)=1.5041109E-2, N(CR)=1.9232487E-3,
    N(NI)=8.5193389E-4, N(CO)=1.696881E-4
POLY_3:
POLY_3: @@... Saving the workspace for the single-point equilibrium
POLY_3: @@                    of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY_3: save TCEX53_c.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: @@ ======================================================================
POLY_3: @@ Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl system
POLY_3: @@ **********************************************************************
POLY_3:
POLY_3: @@... Defining the mapping variables for Pourbaix-diagram mapping:
POLY_3: @@                              pH from  0   to 14
POLY_3: @@                              Eh from -1.2 to 1.5 (V)
POLY_3: s-a-v 1 lnacr(H+1) -32.22994 0 0.5
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 mur(Ze) -150000 200000 5000
   ... the command in full is SET_AXIS_VARIABLE
POLY_3: l-a-v
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: LNACR(H+1)           Min: -32.22994 Max: 0         Inc: 0.5
  Axis No 2: MUR(ZE)              Min: -150000   Max: 200000    Inc: 5000
POLY_3:
POLY_3: @@... Adding the starting points in two or four directions:
POLY_3: @@              (they may be enforced with the option >)
POLY_3: @@ add 1>
POLY_3: @@ add -1>
POLY_3:     add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:     add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: li-in-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  +2  P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2,
    N(CL)=8.5554078E-2, N(FE)=1.5041109E-2, N(CR)=1.9232487E-3,
    N(NI)=8.5193389E-4, N(CO)=1.696881E-4, LNACR(H+1)=-16.118096,
    MUR(ZE)=-4.0143576E-12
 No 2  -2  P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2,
```

```
    N(CL)=8.5554078E-2, N(FE)=1.5041109E-2, N(CR)=1.9232487E-3,
    N(NI)=8.5193389E-4, N(CO)=1.696881E-4, LNACR(H+1)=-16.118096,
    MUR(ZE)=-4.0143576E-12
POLY_3: @?<Hit_return_to_continue>
POLY_3:
POLY_3: @@... Saving the workspace for the Pourbaix-diagram settings
POLY_3: @@                  of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY_3: save TCEX53_d.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: @@... Performing the mapping calculation:
POLY_3: @@    ------------------------------------------------------------
POLY_3: @@    Due to the complexity of aqueous solution model (SIT or HKF),
POLY_3: @@    a complete mapping calculation of the Pourbaix-diagram type
POLY_3: @@    may take a rather long time. Please be patient...
POLY_3: @@    ------------------------------------------------------------
POLY_3: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4

 Phase region boundary   1 at:  -1.612E+01  5.825E+04
     AQUEOUS
     COCR2O4
  ** CR2O3
     HEMATITE
     NIFE2O4
 *** Buffer saved on file: TCEX53_d.POLY3
 Calculated..           34  equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:  -3.223E+01 -8.807E+03
     AQUEOUS
     COCR2O4
  ** CR2O3
     HEMATITE
     NIFE2O4
 Calculated.           38  equilibria

 Phase region boundary   3 at:  -1.404E+01  6.628E+04
     AQUEOUS
     COCR2O4
  ** CR2O3
     HEMATITE
  ** NIFE2O4

 Phase region boundary   4 at:  -1.404E+01  6.628E+04
     AQUEOUS
     COCR2O4
  ** CR2O3
     HEMATITE
 Calculated.            7  equilibria

  .
  .
  .

 Phase region boundary 129 at:  -1.612E+01  5.825E+04
     AQUEOUS#1
     COCR2O4
  ** CR2O3
     HEMATITE
     NIFE2O4
 Calculated.            6  equilibria
 Terminating at known equilibrium
```

```
 Phase region boundary 130 at:  -1.612E+01 -1.748E+03
     AQUEOUS#1
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated..           34  equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

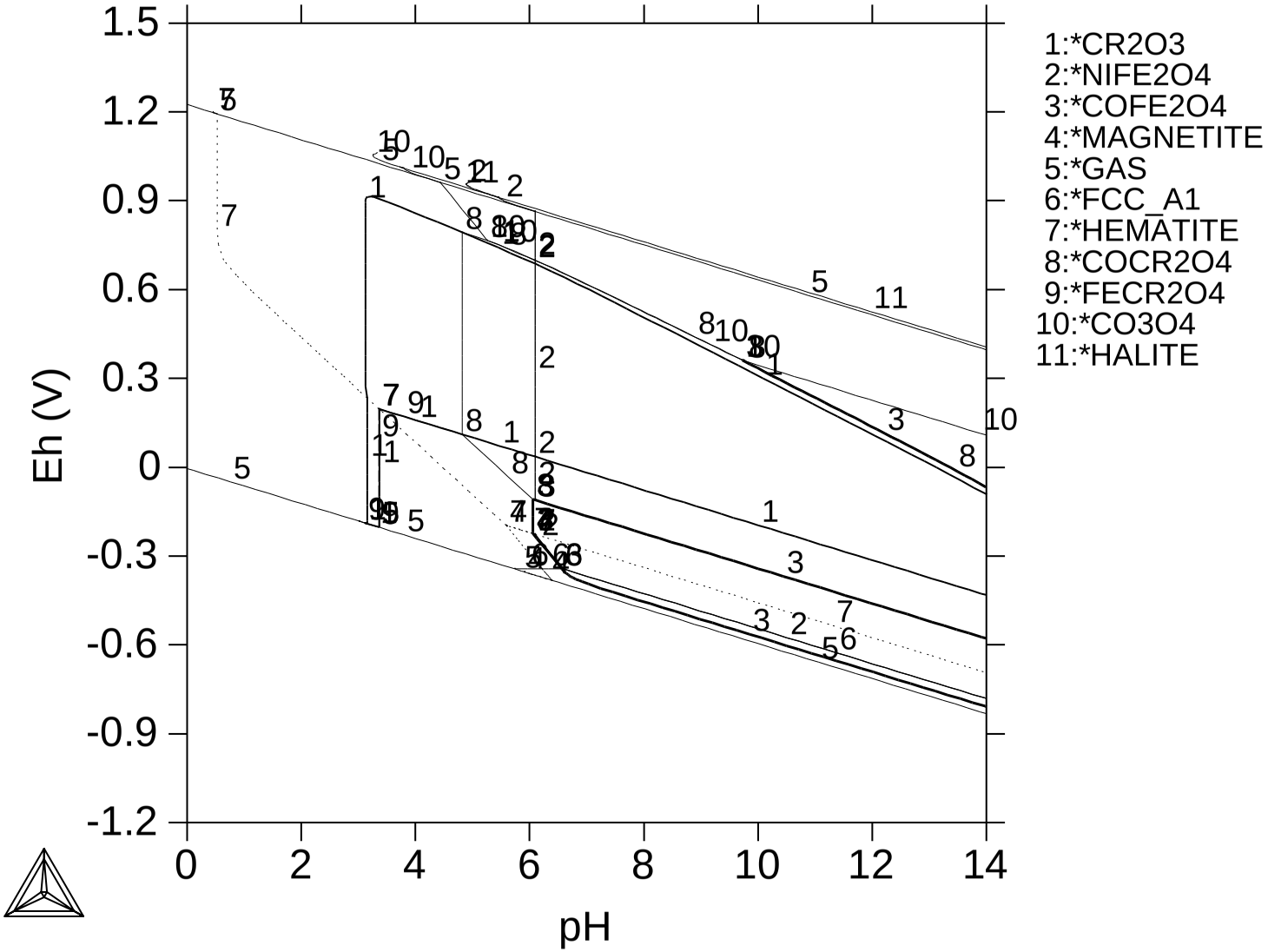
 Phase region boundary 131 at:  -1.612E+01 -1.748E+03
     AQUEOUS#1
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated.            6  equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: TCEX53_d.POLY3
 CPU time for mapping        4195  seconds
POLY_3:
POLY_3: @@... Plotting the calculated Pourbaix diagram (& many others):
POLY_3: @@    ------------------------------------------------------------
POLY_3: post
  POLY-3 POSTPROCESSOR VERSION 3.2 , last update 2002-12-01

 Setting automatic diagram axis

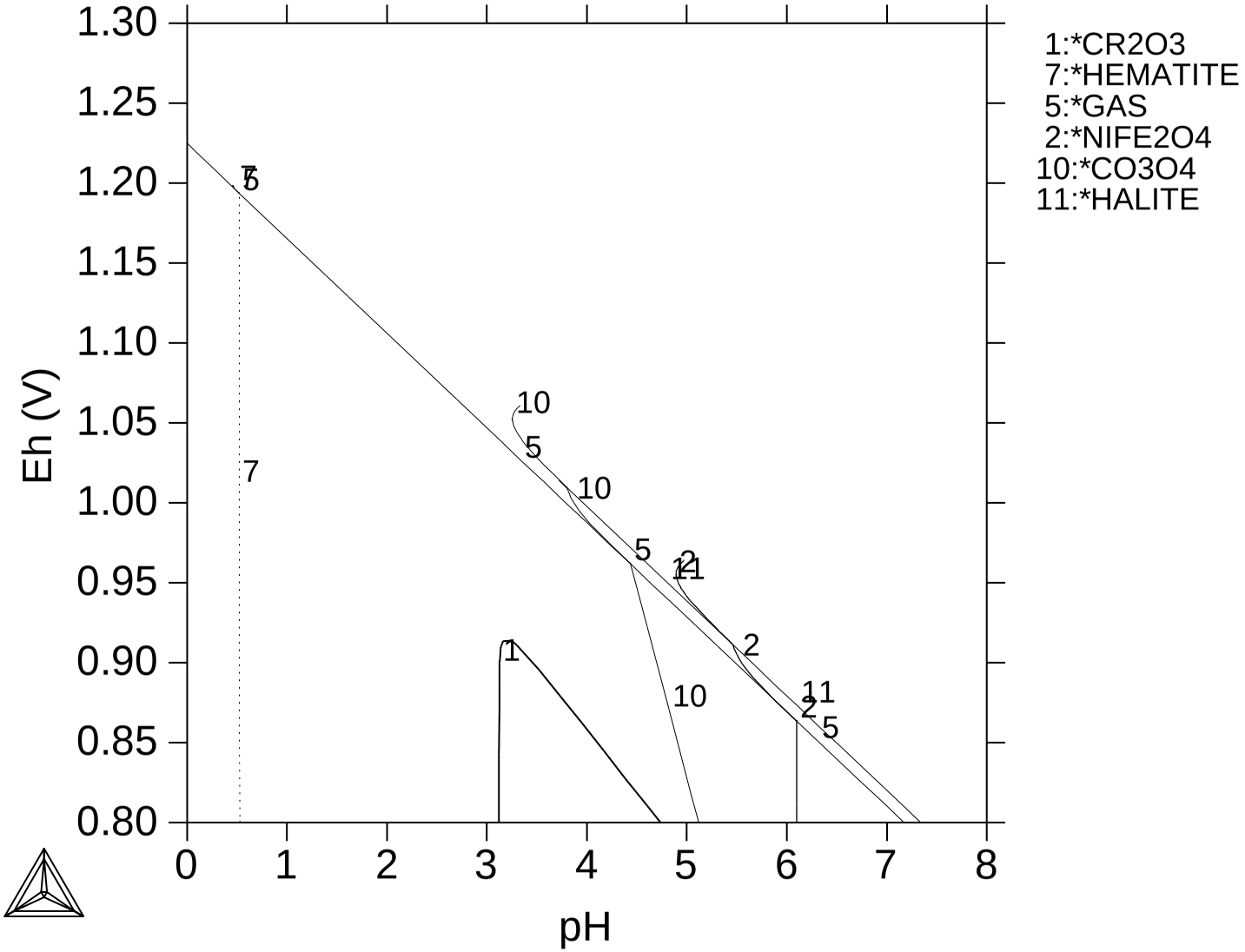
POST: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED CONSTANTS
    AH2O=55.508435, RNF=96485.309, ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1) )
    TEMP_C=T-273.15
POST: @?<Hit_return_to_continue>
POST:
POST: s-d-a x pH
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n pH
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-s-s x n 0 14
   ... the command in full is SET_SCALING_STATUS
POST: s-d-a y Eh
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text y n Eh (V)
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-s-s y n -1.0 1.5
   ... the command in full is SET_SCALING_STATUS
POST: s-t-m-s y
   ... the command in full is SET_TRUE_MANUAL_SCALING
  TRUE MANUAL SCALING SET FOR Y-AXIS
POST: s-l-c e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-font , .32
   ... the command in full is SET_FONT
 CURRENT FONT: Cartographic Roman
 NEW FONT: Cartographic Roman
POST: s-title TCCS Example 53-a
   ... the command in full is SET_TITLE
POST: pl,,,
   ... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
 The composition set AQUEOUS#3 created from the store file
POST: make TCEX53.EXP y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: @?<Hit_return_to_continue>
POST:
POST: s-s-s x n 0 8
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n .8 1.3
```

... the command in full is SET_SCALING_STATUS
POST: **s-title TCCS Example 53-b**
... the command in full is SET_TITLE
POST: **pl,,,**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST: **@?<Hit_return_to_continue>**
POST:
POST: **s-s-s y n -.4 .4**
... the command in full is SET_SCALING_STATUS
POST: **s-title TCCS Example 53-c**
... the command in full is SET_TITLE
POST: **pl,,,**
... the command in full is PLOT_DIAGRAM
PLOTFILE : /SCREEN/:
POST: **@?<Hit_return_to_continue>**
POST:
POST: *@@*
POST: *@@ **
POST: @@ From the same mapping calculations, one may plot many more diagrams,
POST: @@   using various X-Y axis variables (for such purposes, it is very
POST: @@   convenient to use pre-defined symbols as listed at the end of
POST: @@   this MACRO file).
POST: @@ **
POST: @@*
POST:
POST: **SET-INTER**
... the command in full is SET_INTERACTIVE_MODE
POST:POST:POST: CPU time   4208 seconds

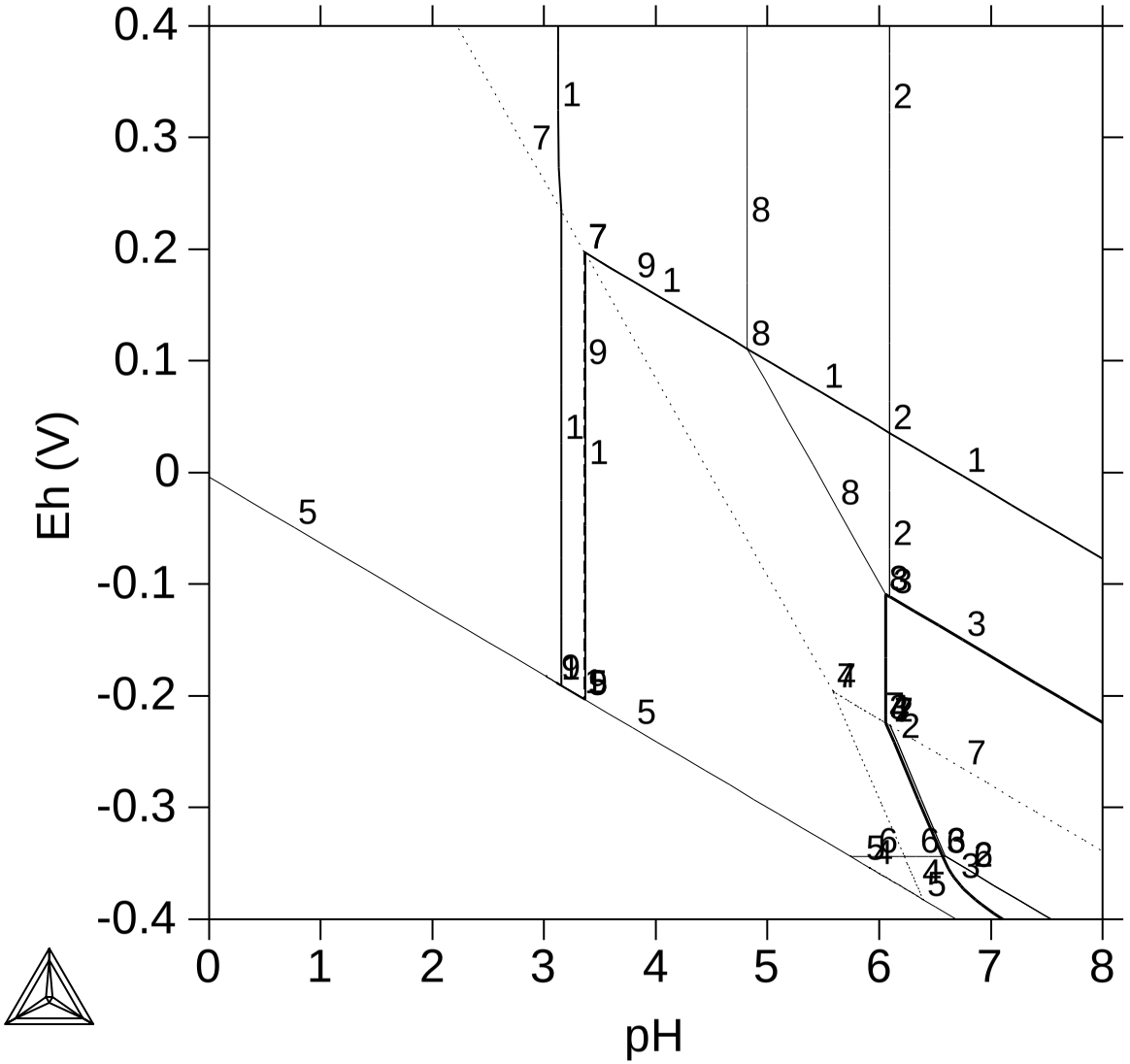
THERMO-CALC (2009.05.19:10.17) :TCCS Example 53-a
DATABASE:PAQ2
P=1E5, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.55541E-2,
N(FE)=1.50411E-2, N(CR)=1.92325E-3, N(NI)=8.51934E-4, N(CO)=1.69688E-4;



THERMO-CALC (2009.05.19:10.16) :TCCS Example 53-b
DATABASE:PAQ2
P=1E5, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.55541E-2,
N(FE)=1.50411E-2, N(CR)=1.92325E-3, N(NI)=8.51934E-4, N(CO)=1.69688E-4;



THERMO-CALC (2009.05.19:10.09) :TCCS Example 53-c
DATABASE:PAQ2
P=1E5, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.55541E-2,
N(FE)=1.50411E-2, N(CR)=1.92325E-3, N(NI)=8.51934E-4, N(CO)=1.69688E-4;



1:*CR2O3
2:*NIFE2O4
3:*COFE2O4
4:*MAGNETITE
5:*GAS
6:*FCC_A1
7:*HEMATITE
8:*COCR2O4
9:*FECR2O4