Thermo-Calc Console Mode Example Macros

Thermo-Calc Version 2020b

Thermo-Calc Software

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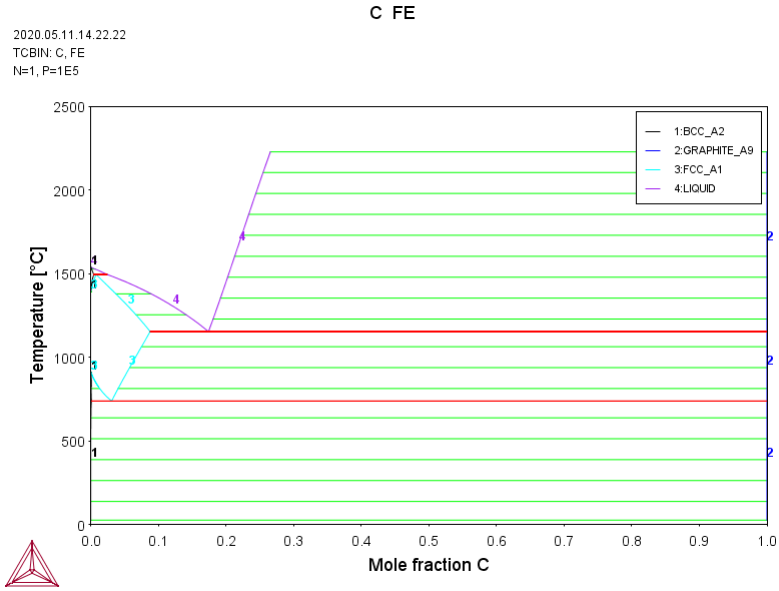
Results

tcex01

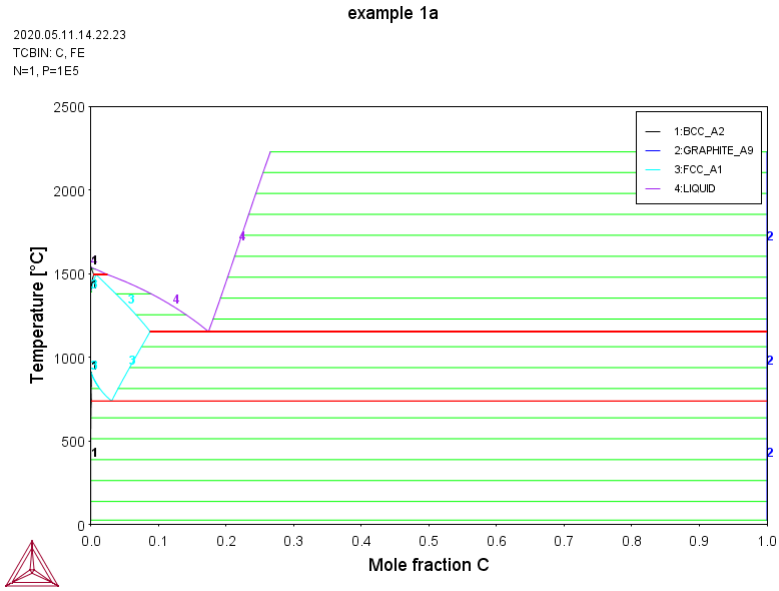
```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex01\tcex01.TCM"
SYS: set-echo
SYS:
SYS: @@ Calculation of the Fe-C binary phase diagram.
SYS:
SYS: @@ This example calculates the binary Fe-C phase
SYS: @@ diagram using the Binary module.
SYS:
SYS: set-log ex01,,,
SYS:
SYS: @@ The log file is set to get command echo.
SYS: @@ The menu is shown by typing a question mark "?"
SYS: ?
   ... the command in full is HELP
 ABOUT                    HP_CALCULATOR            SET_INTERACTIVE_MODE
 BACK                     INFORMATION              SET_LOG_FILE
 CLOSE_FILE               MACRO_FILE_OPEN          SET_PLOT_ENVIRONMENT
 DISPLAY_LICENSE_INFO     OPEN_FILE                SET_POLY_VERSION
 EXIT                     SET_COMMAND_UNITS        SET_TC_OPTIONS
 GOTO_MODULE              SET_ECHO                 SET_TERMINAL
 HELP                     SET_GES_VERSION          STOP_ON_ERROR
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
 FILE SYSTEM ERROR                     37
 *** ERROR  1717 IN MLOPEN: FILE DOES NOT EXIST: c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\help\sysmon.hlp
  ERROR                   1717  RESET
SYS: ?
   ... the command in full is HELP
 ABOUT                    HP_CALCULATOR            SET_INTERACTIVE_MODE
 BACK                     INFORMATION              SET_LOG_FILE
 CLOSE_FILE               MACRO_FILE_OPEN          SET_PLOT_ENVIRONMENT
 DISPLAY_LICENSE_INFO     OPEN_FILE                SET_POLY_VERSION
 EXIT                     SET_COMMAND_UNITS        SET_TC_OPTIONS
 GOTO_MODULE              SET_ECHO                 SET_TERMINAL
 HELP                     SET_GES_VERSION          STOP_ON_ERROR
SYS:
SYS:
SYS:Hit RETURN to continue
SYS: @@ For a binary phase diagram calculation we use the binary module
SYS: go
   ... the command in full is GOTO_MODULE
MODULE NAME: ?
 NO SUCH MODULE, USE ANY OF THESE:
 SYSTEM_UTILITIES
 GIBBS_ENERGY_SYSTEM
 TABULATION_REACTION
 POLY_3
 DICTRA_MONITOR
 BINARY_DIAGRAM_EASY
 DATABASE_RETRIEVAL
 DIC_PARROT
 REACTOR_SIMULATOR_3
 PARROT
 POTENTIAL_DIAGRAM
 SCHEIL_SIMULATION
 OLD_SCHEIL_SIM
 POURBAIX_DIAGRAM
 TERNARY_DIAGRAM
MODULE NAME: BIN
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC  Binary Solutions  v1.1

 VA                       /-  DEFINED
 BCC_B2                   FCC_L12                  FCC_L102
 D021_HCP  REJECTED
First element: fe
Second element: c
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase-Diagram
   ... the command in full is REJECT
 VA                       /-  DEFINED
 BCC_B2                   FCC_L12                  FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES .....
   ... the command in full is DEFINE_ELEMENTS
 C                        FE  DEFINED
 LIQUID:L                 IONIC_LIQUID:Y           FCC_A1
 BCC_A2                   A2_BCC                   HCP_A3
 HCP_ZN                   DIAMOND_A4               GRAPHITE_A9
 CBCC_A12                 CUB_A13                  B2_FEPD
 C14_LAVES                C15_LAVES                D011_CEMENTITE
 D82_FEZN_GAMMA           L12_FEPD3                AL5FE4
 FE3AS2                   FEZN4                    FEZN_DELTA
```

```
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 BCC_A2  RESTORED
 D011_CEMENTITE  RESTORED
 GRAPHITE_A9  RESTORED
 DIAMOND_A4  RESTORED
   ... the command in full is GET_DATA
14:22:14,191 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'P Gustafson, Scan J Metall 14(1985) p 259-267; C-Fe'
 -OK-
   ... the command in full is SET_CONDITION
   ... 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

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

 Organizing start points

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   9.944E-01  1.100E+03
     BCC_A2
  ** FCC_A1
 Calculated.                      5 equilibria

 Phase region boundary   2 at:   9.838E-01  1.011E+03
     BCC_A2
  ** FCC_A1
  ** GRAPHITE_A9

 Phase region boundary   3 at:   4.996E-01  1.011E+03
     BCC_A2
  ** GRAPHITE_A9
 Calculated..                     30 equilibria
 Terminating at axis limit.

 Phase region boundary   4 at:   4.845E-01  1.011E+03
     FCC_A1
  ** GRAPHITE_A9
 Calculated.                     18 equilibria

 Phase region boundary   5 at:   4.561E-01  1.427E+03
  ** LIQUID
     FCC_A1
  ** GRAPHITE_A9

 Phase region boundary   6 at:   8.690E-01  1.427E+03
  ** LIQUID
     FCC_A1
 Calculated.                     15 equilibria

 Phase region boundary   7 at:   9.840E-01  1.768E+03
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary   8 at:   9.939E-01  1.768E+03
  ** BCC_A2
     FCC_A1
 Calculated                     25 equilibria

 Phase region boundary   9 at:   9.858E-01  1.768E+03
     LIQUID
  ** BCC_A2
 Calculated                     20 equilibria

 Phase region boundary  10 at:   4.129E-01  1.427E+03
  ** LIQUID
     GRAPHITE_A9
 Calculated..                     44 equilibria
 Terminating at axis limit.

 Phase region boundary  11 at:   9.841E-01  1.011E+03
     BCC_A2
  ** FCC_A1
 Calculated                     25 equilibria

 Phase region boundary  12 at:   9.944E-01  1.100E+03
     BCC_A2
  ** FCC_A1
 Calculated                     16 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\BINARY_002.POLY3
 CPU time for mapping                    4 seconds
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes
```

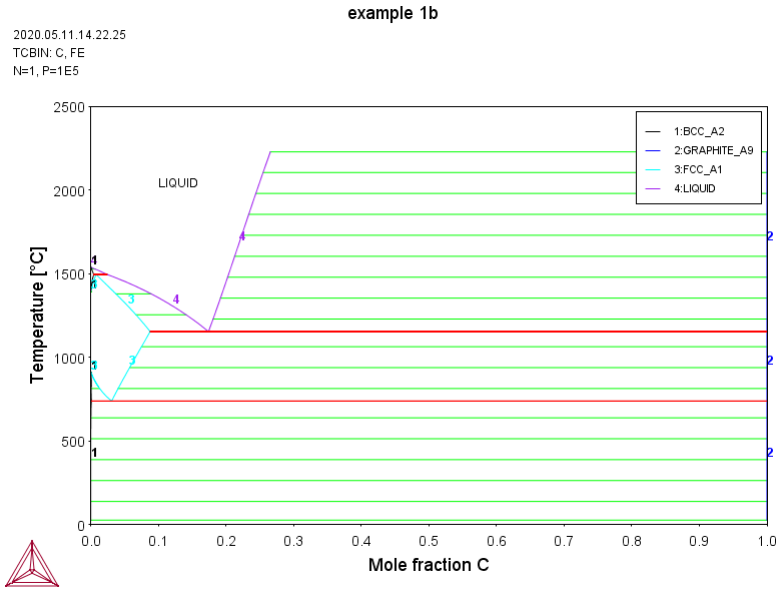
```
 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

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



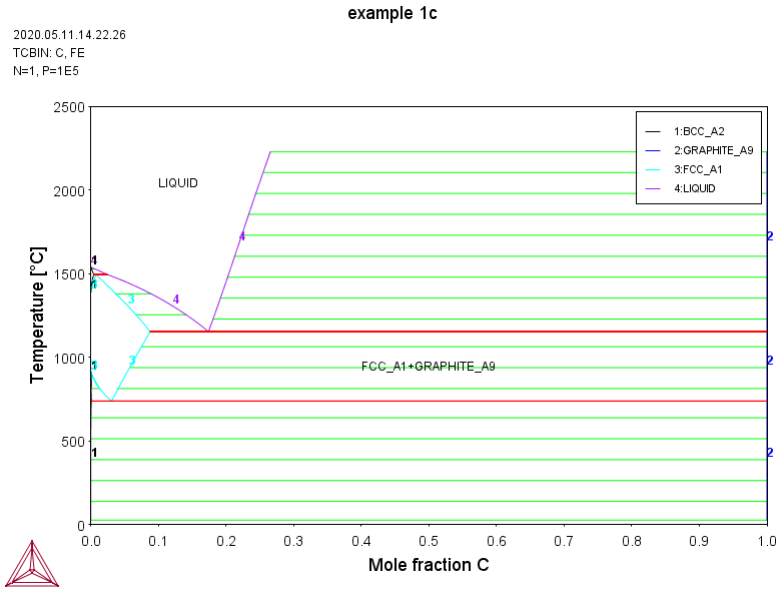

```
POST:
POST:Hit RETURN to continue
POST:
POST: set-title example 1a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ By default no label is given, the user must specify it.
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           630 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: LIQUID
Text size: /.36/:
POST: set-title example 1b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

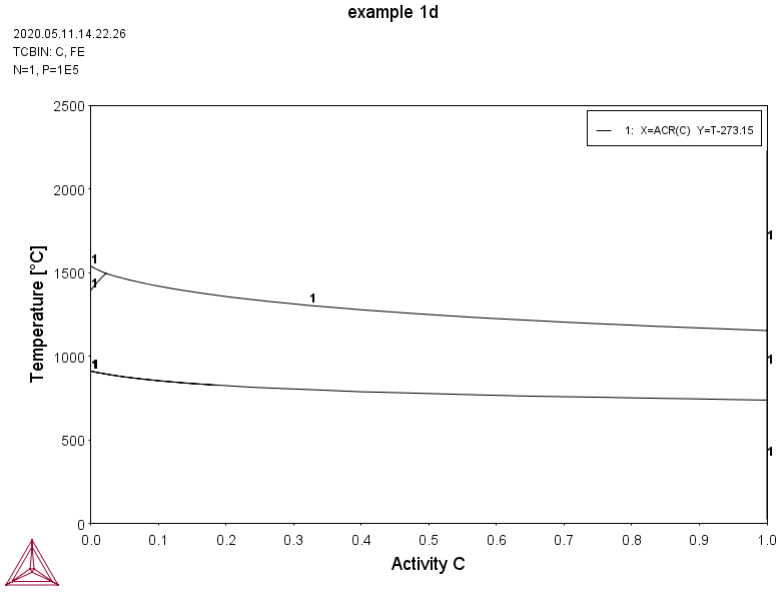



```
POST:
POST:
POST:Hit RETURN to continue
POST: add .4 900
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/: Y
 Automatic labelling not always possible
 Using global minimization procedure
Calculated           630 grid points in              0 s
Found the set of lowest grid points in               0 s
 Calculated POLY solution       0 s, total time      0  s
 Stable phases are: FCC_A1+GRAPHITE_A9
Text size: /.36/:
POST: set-title example 1c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

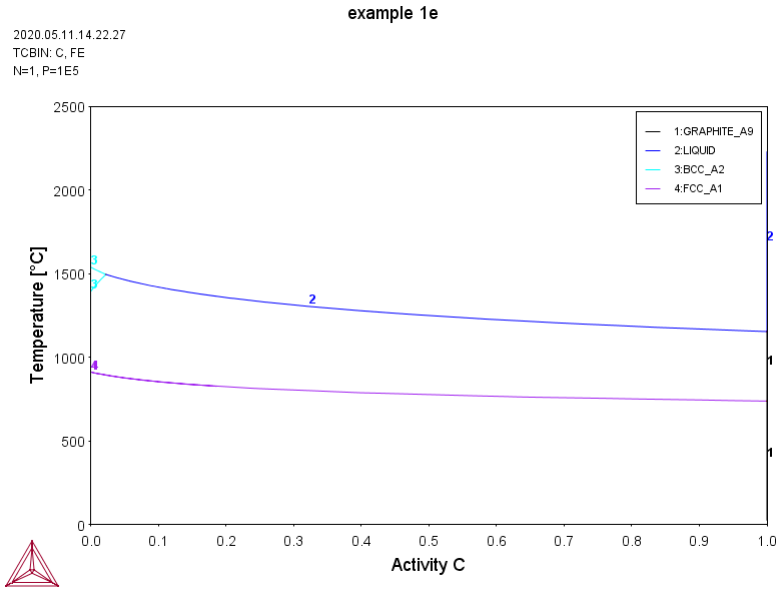



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ This is the stable phase diagram with graphite and no cementite.
POST: @@ In Thermo-Calc all relevant data from the calculation of the diagram is saved
POST: @@ and it is possible to plot the same diagram using other thermodynamic
POST: @@ quantities, for example replace the carbon composition with its activity
POST: @@ Find out the commands in the post processor by entering ?
POST: ?
   ... the command in full is HELP
 ADD_LABEL_TEXT            PLOT_DIAGRAM              SET_INTERACTIVE_MODE
 APPEND_EXPERIMENTAL_DATA  PRINT_DIAGRAM             SET_LABEL_CURVE_OPTION
 BACK                      QUICK_EXPERIMENTAL_PLOT   SET_PLOT_FORMAT
 CHANGE_LEGEND             REINITIATE_PLOT_SETTINGS  SET_PLOT_OPTIONS
 CREATE_3D_PLOTFILE        RESTORE_PHASE_IN_PLOT     SET_PLOT_SIZE
 DUMP_DIAGRAM              SELECT_PLOT               SET_PREFIX_SCALING
 ENTER_SYMBOL              SET_AXIS_LENGTH           SET_RASTER_STATUS
 EXIT                      SET_AXIS_PLOT_STATUS      SET_REFERENCE_STATE
 FIND_LINE                 SET_AXIS_TEXT_STATUS      SET_SCALING_STATUS
 HELP                      SET_AXIS_TYPE             SET_TIC_TYPE
 LIST_DATA_TABLE           SET_COLOR                 SET_TIELINE_STATUS
 LIST_PLOT_SETTINGS        SET_CORNER_TEXT           SET_TITLE
 LIST_SYMBOLS              SET_DIAGRAM_AXIS          SET_TRUE_MANUAL_SCALING
 MAKE_EXPERIMENTAL_DATAFI  SET_DIAGRAM_TYPE          SUSPEND_PHASE_IN_PLOT
 MODIFY_LABEL_TEXT         SET_FONT                  TABULATE
POST: @@ The command to set axis for the diagram is SET-DIAGRAM-AXIS
POST: s-d-a x
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
 FILE SYSTEM ERROR IN FILHLP
 ERROR                    1717  READING HELP FILE
```

```
VARIABLE : ac
FOR COMPONENT : c
POST: set-title example 1d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ The diagram stops at unit activity which represent graphite.
POST: @@ The labels disappear when one sets a new diagram axis because they
POST: @@ are relative to the axis values, not the axis quantities.
POST: @@
POST: @@ An easier way to identify the stable phases is to use
POST: @@ the command set-label
POST: set-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: ?
 THE OPTIONS MEANS:
 A     LIST STABLE PHASES ALONG LINE
 B     AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
 C     LIST AXIS QUANTITIES
 D     AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
 E     AS B WITH CHANGING COLORS
 F     AS D WITH CHANGING COLORS
 N     NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: B
POST: set-title example 1e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ The metastable diagram, with cementite, can also be calculated but then
POST: @@ one must do some manipulations in POLY. We can use the data
POST: @@ we already retrieved from the database.
POST: back
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
SYS: go p-3
   ... the command in full is GOTO_MODULE
POLY:
POLY: @@ The BIN module has used the poly-3 workspace to calculate the
POLY: @@ diagram. We have all data available here. The workspace has been
POLY: @@ saved on a file and we can read this back with the command READ.
```

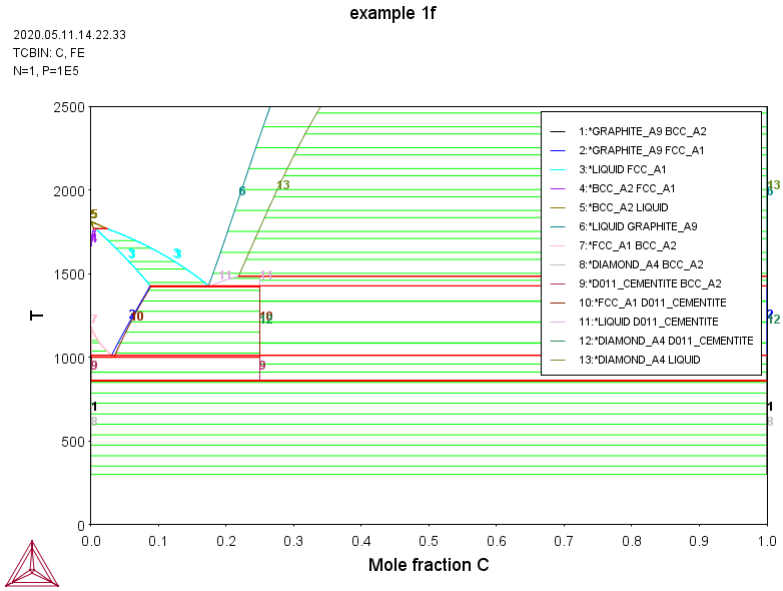
```
POLY:
POLY: read,,,
   ... the command in full is READ_WORKSPACES
POLY:
POLY: @@ There are many commands in the POLY module. This enables you
POLY: @@ to calculate almost any kind of equilibrium and diagram.
POLY: @@ With the ? you can list all commands
POLY: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  GOTO_MODULE              REINITIATE_MODULE
 ADVANCED_OPTIONS         HELP                     SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  INFORMATION              SELECT_EQUILIBRIUM
 BACK                     LIST_AXIS_VARIABLE       SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_CONDITIONS          SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_EQUILIBRIUM         SET_CONDITION
 COMPUTE_TRANSITION       LIST_INITIAL_EQUILIBRIA  SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_STATUS              SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_SYMBOLS             SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
 DEFINE_MATERIAL          MACRO_FILE_OPEN          SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MAKE_COMPONENT_ENTERED   SET_START_VALUE
 DELETE_SYMBOL            MAKE_COMPONENT_SUSPENDED SHOW_VALUE
 ENTER_SYMBOL             MAP                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       POST                     TABULATE
 EXIT                     READ_WORKSPACES
POLY:
POLY:Hit RETURN to continue
POLY: @@ Get more command information with the HELP command
POLY: help
COMMAND: list-status
 *** ERROR    37 IN FILDOC: FILE SYSTEM ERROR
POLY:Hit RETURN to continue
POLY: @@ General information can be obtained using the INFORMATION command
POLY: INFO
   ... the command in full is INFORMATION
 FILE SYSTEM ERROR                     37
POLY:
POLY: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  GOTO_MODULE              REINITIATE_MODULE
 ADVANCED_OPTIONS         HELP                     SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  INFORMATION              SELECT_EQUILIBRIUM
 BACK                     LIST_AXIS_VARIABLE       SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_CONDITIONS          SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_EQUILIBRIUM         SET_CONDITION
 COMPUTE_TRANSITION       LIST_INITIAL_EQUILIBRIA  SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_STATUS              SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_SYMBOLS             SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
 DEFINE_MATERIAL          MACRO_FILE_OPEN          SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MAKE_COMPONENT_ENTERED   SET_START_VALUE
 DELETE_SYMBOL            MAKE_COMPONENT_SUSPENDED SHOW_VALUE
 ENTER_SYMBOL             MAP                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       POST                     TABULATE
 EXIT                     READ_WORKSPACES
POLY: state
 No such command, use ?
POLY:
POLY:Hit RETURN to continue
POLY: @@ List the current equilibrium by
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: ?
 FILE SYSTEM ERROR IN FILHLP
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCBIN

 Conditions:
 N=1, P=1E5, X(FE)=0.99, T=1100
 DEGREES OF FREEDOM 0

 Temperature   1100.00 K (   826.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.54086E+01
 Total Gibbs energy -4.90502E+04,  Enthalpy  3.18534E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.0000E-02  2.1677E-03 1.8555E-01 -1.5406E+04 GRAPHITE
 FE                      9.9000E-01  9.9783E-01 9.9957E-01 -3.9762E+00 BCC_A2

 FCC_A1                     Status ENTERED     Driving force  0.0000E+00
 Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.97662E-01  C   2.33819E-03

 BCC_A2                     Status ENTERED     Driving force  0.0000E+00
 Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.99907E-01  C   9.33835E-05
POLY:Hit RETURN to continue
POLY: @@ The actual conditions are listed by the list-equil command but
POLY: @@ can be obtained also by
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 N=1, P=1E5, X(FE)=0.99, T=1100
 DEGREES OF FREEDOM 0
POLY:
POLY:Hit RETURN to continue
POLY: @@ The meaning of the state variables T, P, X, N  and many others
POLY: @@ are explained by the INFO command
POLY: INFO
   ... the command in full is INFORMATION
 FILE SYSTEM ERROR                     37
POLY: state
 No such command, use ?
POLY:
POLY:Hit RETURN to continue
POLY: @@ The use of state variables as conditions is the key to the
POLY: @@ flexibility of Thermo-Calc. Each condition is set independently and
POLY: @@ any condition can be set as an axis variable.
POLY: @@
POLY: @@ Now we just want to take away the graphite in order to calculate the
POLY: @@ metastable Fe-C diagram with cementite. We can list all phases with the
POLY: @@ LIST_STATUS command
POLY: l-st
   ... the command in full is LIST_STATUS
```

```
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)            P(Pa)
 VA                       ENTERED   SER
 C                        ENTERED   GRAPHITE_A9    *               100000
 FE                       ENTERED   BCC_A2         *               100000
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    9.246266E-01
 BCC_A2                   ENTERED      0.000000E+00    7.537335E-02
 D011_CEMENTITE           ENTERED     -4.153716E-01    0.000000E+00
 LIQUID                   ENTERED     -4.668963E-01    0.000000E+00
 GRAPHITE_A9              ENTERED     -1.684424E+00    0.000000E+00
 DIAMOND_A4               ENTERED     -2.386932E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 C    ENTERED    C3   ENTERED    FE   ENTERED    VA   ENTERED
 C1   ENTERED    C4   ENTERED    FE+2 ENTERED    VA-2 ENTERED
 C2   ENTERED    C5   ENTERED    FE+3 ENTERED    VA-4 ENTERED
POLY:Hit RETURN to continue
POLY: @@ The status is changed with the CHANGE_STATUS command
POLY: ch-st
   ... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): ?
 FILE SYSTEM ERROR IN FILHLP
Phase name(s): gra
Status: /ENTERED/: sus
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)            P(Pa)
 VA                       ENTERED   SER
 C                        ENTERED   GRAPHITE_A9    *               100000
 FE                       ENTERED   BCC_A2         *               100000
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    9.246266E-01
 BCC_A2                   ENTERED      0.000000E+00    7.537335E-02
 D011_CEMENTITE           ENTERED     -4.153716E-01    0.000000E+00
 LIQUID                   ENTERED     -4.668963E-01    0.000000E+00
 DIAMOND_A4               ENTERED     -2.386932E+00    0.000000E+00
 SUSPENDED PHASES:
 GRAPHITE_A9
 *** STATUS FOR ALL SPECIES
 C    ENTERED    C3   ENTERED    FE   ENTERED    VA   ENTERED
 C1   ENTERED    C4   ENTERED    FE+2 ENTERED    VA-2 ENTERED
 C2   ENTERED    C5   ENTERED    FE+3 ENTERED    VA-4 ENTERED
POLY:Hit RETURN to continue
POLY: @@ Note that the graphite is listed as suspended this time.
POLY: @@ Now try to calculate the equilibrium without graphite.
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           629 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: @@ A number of ,,, after a command means to accept default values.
POLY: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCBIN

 Conditions:
 N=1, P=1E5, X(FE)=0.99, T=1100
 DEGREES OF FREEDOM 0

 Temperature   1100.00 K (   826.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.54086E+01
 Total Gibbs energy -4.90502E+04,  Enthalpy  3.18534E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        1.0000E-02  2.1677E-03 1.8555E-01 -1.5406E+04 GRAPHITE
 FE                       9.9000E-01  9.9783E-01 9.9957E-01 -3.9762E+00 BCC_A2

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.97662E-01  C   2.33819E-03

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.99907E-01  C   9.33835E-05
POLY:Hit RETURN to continue
POLY: @@ It may seem surprising that diamond is stable but the total mole fraction
POLY: @@ of iron is less than 0.5, so we are on the carbon rich side
POLY: @@ of cementite, and it is reasonable.
POLY:
POLY: @@ Now try to map the metastable diagram
POLY: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

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

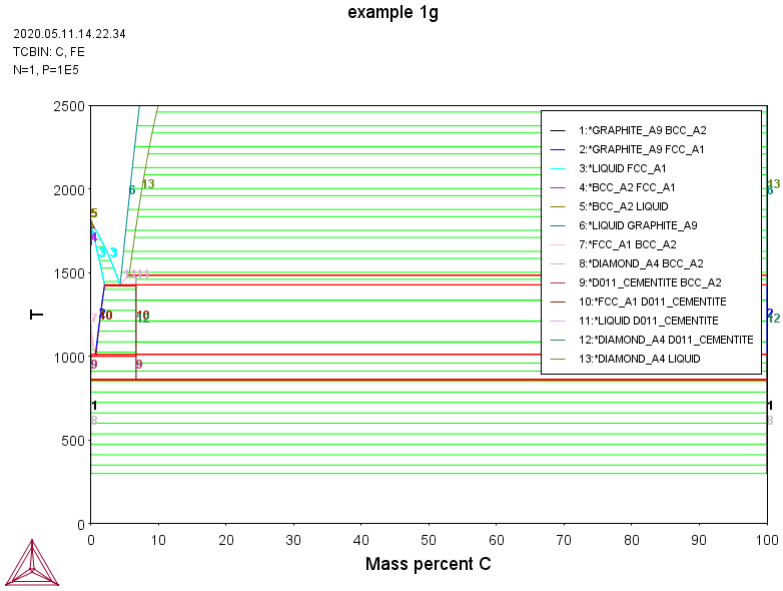
```
Generating start point  10
Working hard
Generating start point  11
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28
Generating start point  29
Generating start point  30
Working hard
Generating start point  31
Generating start point  32

Phase region boundary   1 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2 equilibria
Terminating at axis limit.

Phase region boundary   2 at:   5.000E-01  3.000E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                      24 equilibria

Phase region boundary   3 at:   4.999E-01  8.605E+02
    BCC_A2
 ** D011_CEMENTITE
 ** DIAMOND_A4

Phase region boundary   4 at:   8.749E-01  8.605E+02
    BCC_A2
 ** D011_CEMENTITE
Calculated.                       7 equilibria

Phase region boundary   5 at:   8.746E-01  9.998E+02
    BCC_A2
 ** D011_CEMENTITE
 ** FCC_A1

Phase region boundary   6 at:   9.823E-01  9.998E+02
    BCC_A2
 ** FCC_A1
Calculated                      23 equilibria

Phase region boundary   7 at:   8.578E-01  9.998E+02
    D011_CEMENTITE
 ** FCC_A1
Calculated.                      18 equilibria

Phase region boundary   8 at:   8.354E-01  1.422E+03
 ** LIQUID
    D011_CEMENTITE
 ** FCC_A1

Phase region boundary   9 at:   7.872E-01  1.422E+03
 ** LIQUID
    D011_CEMENTITE
Calculated.                       5 equilibria

Phase region boundary  10 at:   7.657E-01  1.484E+03
 ** LIQUID
    D011_CEMENTITE
 ** DIAMOND_A4

Phase region boundary  11 at:   3.750E-01  1.484E+03
    D011_CEMENTITE
 ** DIAMOND_A4
Calculated.                      26 equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   3.907E-01  1.484E+03
    LIQUID
 ** DIAMOND_A4
Calculated..                      42 equilibria
Terminating at axis limit.

Phase region boundary  13 at:   8.678E-01  1.422E+03
 ** LIQUID
    FCC_A1
Calculated.                      15 equilibria

Phase region boundary  14 at:   9.840E-01  1.768E+03
 ** LIQUID
 ** BCC_A2
    FCC_A1

Phase region boundary  15 at:   9.939E-01  1.768E+03
 ** BCC_A2
    FCC_A1
Calculated                      25 equilibria

Phase region boundary  16 at:   9.858E-01  1.768E+03
    LIQUID
 ** BCC_A2
Calculated                      20 equilibria

Phase region boundary  17 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                      24 equilibria
Terminating at known equilibrium
```

```
Phase region boundary  18 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  19 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                      24 equilibria
Terminating at known equilibrium

Phase region boundary  20 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  21 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                      24 equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  23 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                      24 equilibria
Terminating at known equilibrium

Phase region boundary  24 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  25 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                      24 equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  27 at:   5.000E-01  3.100E+02
    BCC_A2
 ** DIAMOND_A4
Calculated.                      24 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   3.750E-01  1.037E+03
 ** D011_CEMENTITE
    DIAMOND_A4
Calculated.                       9 equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   3.750E-01  1.037E+03
 ** D011_CEMENTITE
    DIAMOND_A4
Calculated.                      19 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   9.877E-01  1.037E+03
    BCC_A2
 ** FCC_A1
Calculated.                       3 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   9.877E-01  1.037E+03
    BCC_A2
 ** FCC_A1
Calculated                      23 equilibria

Phase region boundary  32 at:   3.754E-01  1.763E+03
    LIQUID
 ** DIAMOND_A4
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   3.754E-01  1.763E+03
    LIQUID
 ** DIAMOND_A4
Calculated..                      31 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  34 at:   9.820E-01  1.763E+03
    LIQUID
 ** FCC_A1
Calculated.                      15 equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   9.820E-01  1.763E+03
    LIQUID
 ** FCC_A1
Calculated.                       2 equilibria
Terminating at known equilibrium

Phase region boundary  36 at:   3.306E-01  2.490E+03
    LIQUID
 ** DIAMOND_A4
```

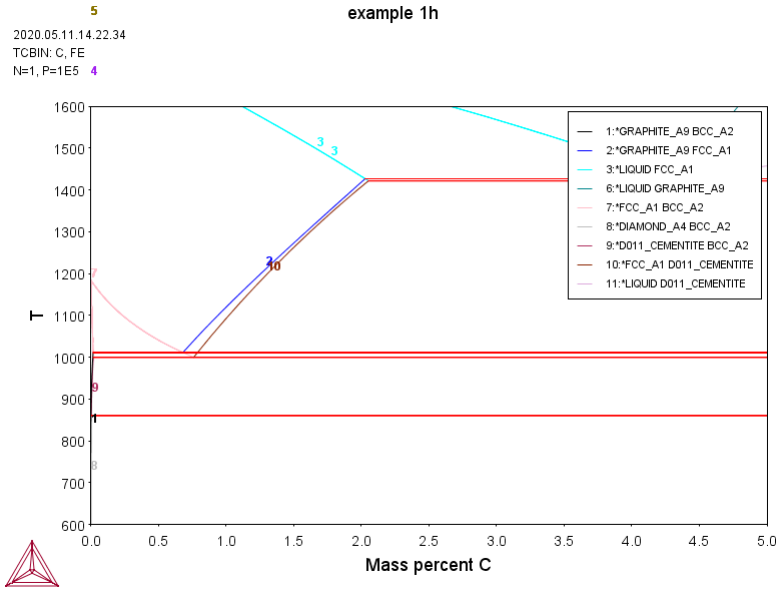
```
 Calculated.                      42 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_A4
 Calculated..                       2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  38 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_A4
 Calculated.                      42 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_A4
 Calculated..                       2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  40 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_A4
 Calculated.                      42 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_A4
 Calculated..                       2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  42 at:   3.317E-01  2.475E+03
     LIQUID
  ** DIAMOND_A4
 Calculated..                       2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  43 at:   3.317E-01  2.475E+03
     LIQUID
  ** DIAMOND_A4
 Calculated.                      41 equilibria
 Terminating at known equilibrium

 Phase region boundary  44 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_A4
 Calculated.                      42 equilibria
 Terminating at known equilibrium

 Phase region boundary  45 at:   3.306E-01  2.490E+03
     LIQUID
  ** DIAMOND_A4
 Calculated..                       2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

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

 Phase region boundary  47 at:   9.941E-01  1.794E+03
     LIQUID
  ** BCC_A2
 Calculated                      12 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\BINARY_002.POLY3
 CPU time for mapping                     3 seconds
POLY:
POLY: post
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x m-f C
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-tieline
   ... the command in full is SET_TIELINE_STATUS
PLOTTING EVERY TIE-LINE NO /5/: 5
POST:
POST: set-title example 1f
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



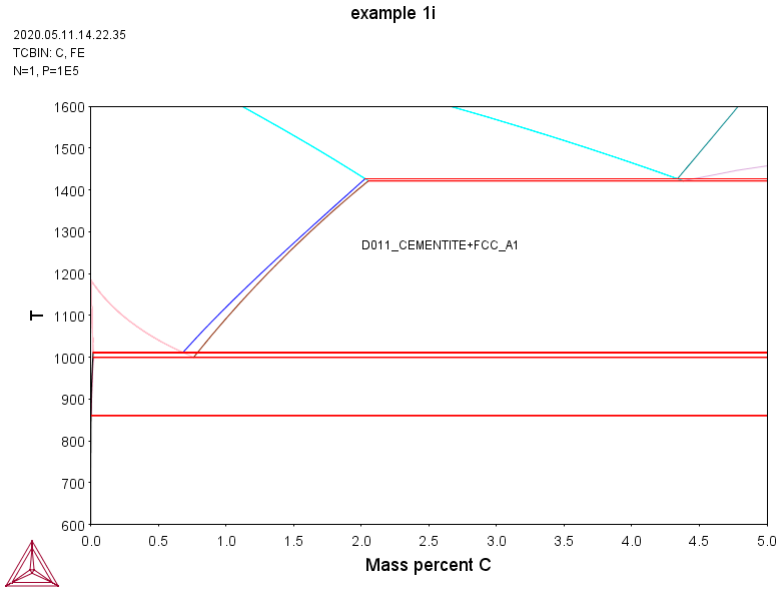

```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ The previous stable diagram is also plotted. The reason is that
POST: @@ we never removed it from the workspace. (It can be done with a SAVE
POST: @@ command. Search the online help to read more about this command).
POST:
POST: @@ It may be surprising to find that diamond is more stable than
POST: @@ cementite at low temperatures. However, diamonds are never
POST: @@ found in steel as graphite forms 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 : ?
 FILE SYSTEM ERROR IN FILHLP
 ERROR                    1717  READING HELP FILE
VARIABLE : w-p
FOR COMPONENT : c
POST: set-title example 1g
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ The tie-lines now obscure the diagram. Remove these and
POST: @@ also change the scale of the x and y axis
POST: s-t-s 0
   ... the command in full is SET_TIELINE_STATUS
POST: s-s x n 0 5
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 600 1600
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 1h
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

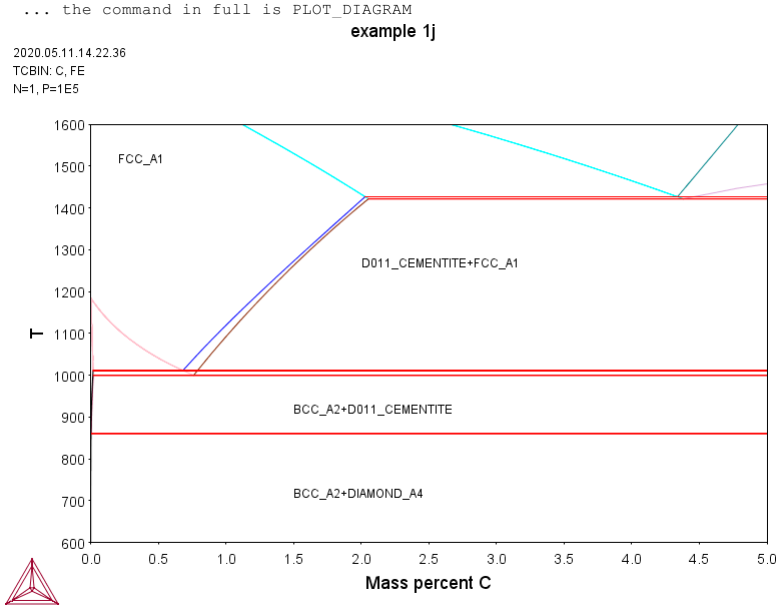



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Finally add some labels
POST: set-lab n
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: add 2 1250
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated           629 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: D011_CEMENTITE+FCC_A1
Text size: /.36/:
POST: set-title example 1i
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

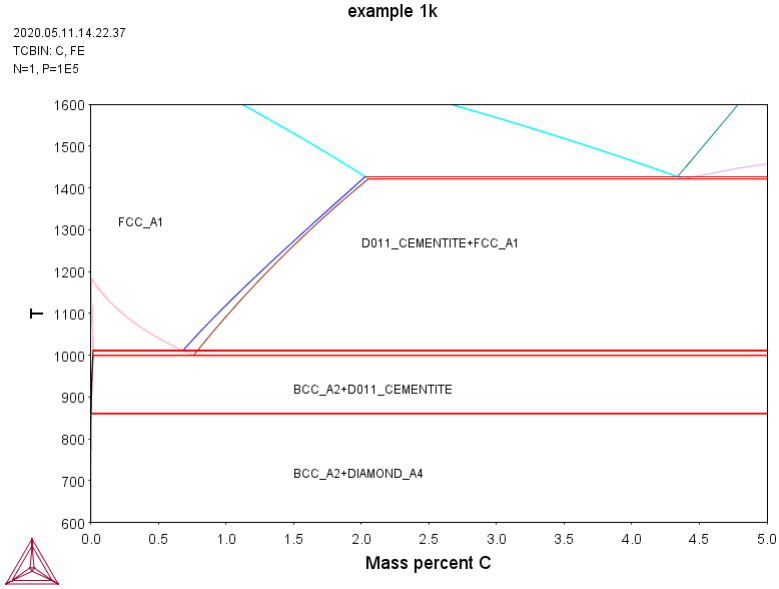



```
POST:
POST:
POST:Hit RETURN to continue
POST: add 1.5 900
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated           629 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_A2+D011_CEMENTITE
Text size: /.36/:
POST: add 1.5 700
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated           629 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_A2+DIAMOND_A4
Text size: /.36/:
POST: add .2 1500
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
```

```
Calculated           629 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: FCC_A1
Text size: /.36/:
POST: set-title example 1j
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ As graphite is suspended, cementite is the stable carbide
POST: @@ so that is the phase that is listed in the two-phase regions.
POST: @@ The label for the FCC region is a bit too high, move it down
POST: modify
   ... the command in full is MODIFY_LABEL_TEXT
 These labels are defined
 No   1 at  2.00000E+00 1.25000E+03 : D011_CEMENTITE+FCC_A1
 No   2 at  1.50000E+00 9.00000E+02 : BCC_A2+D011_CEMENTITE
 No   3 at  1.50000E+00 7.00000E+02 : BCC_A2+DIAMOND_A4
 No   4 at  2.00000E-01 1.50000E+03 : FCC_A1
Which label to modify? /4/:
New X coordinate /.2/: .2
New Y coordinate /1500/: 1300
New text /FCC_A1/:
POST: set-title example 1k
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

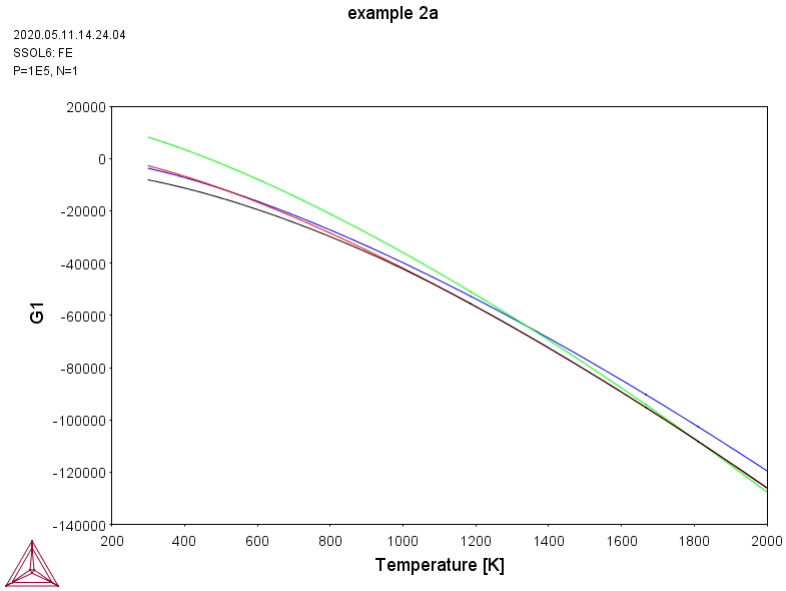



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

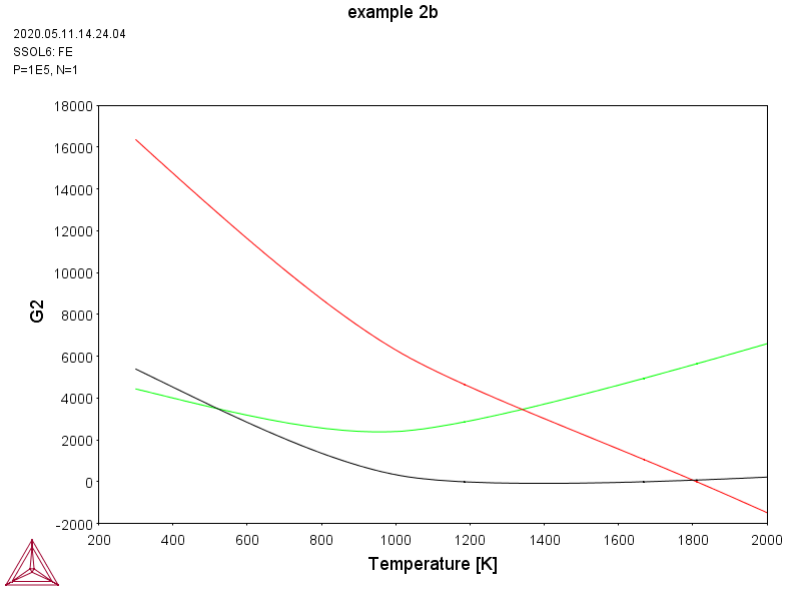
tcex02

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex02\tcex02.TCM.test"
SYS: set-echo
SYS: @@
SYS: @@ Plotting thermodynamic functions
SYS:
SYS: @@ This example shows how to plot thermodynamic
SYS: @@ functions in unary, binary and ternary systems.
SYS: @@ It also involves working with partial derivatives
SYS: @@ and partial quantities.
SYS:
SYS: set-log ex02,,
SYS:
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw ssol6
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Alloy Solutions Database v6.0

 VA  DEFINED
 BCC_B2                  FCC_L12                 FCC_COV
 FCC_AUCU                HCP_ORD  REJECTED
 GAS:G  REJECTED
TDB_SSOL6: @@ Pure Fe is selected as a unary system
TDB_SSOL6: d-sys fe
   ... the command in full is DEFINE_SYSTEM
 FE  DEFINED
TDB_SSOL6: get
   ... the command in full is GET_DATA
14:23:57,403 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 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

  'Benyan Pei, B Bjorkman, B Sundman, and B Jansson: Calphad, 1995, 19(1), 1
      -15. "A thermodynamic assessment of the Iron-Antimony system". >> Fe
      -Sb '
 -OK-
TDB_SSOL6:
TDB_SSOL6: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ In POLY-3 first define a single equilibrium

POLY: s-c t=300,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated            21 grid points in             1 s
POLY: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL6

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

 Temperature    300.00 K (    26.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.58470E+01
 Total Gibbs energy -8.18407E+03,  Enthalpy  4.59751E+01,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 FE                      1.0000E+00  1.0000E+00 3.7589E-02 -8.1841E+03 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.5847E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  1.00000E+00
POLY:
POLY:Hit RETURN to continue
POLY: @@ Set T as an axis variable
POLY: 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: @@ Save the macro to be able to come back to this point
```

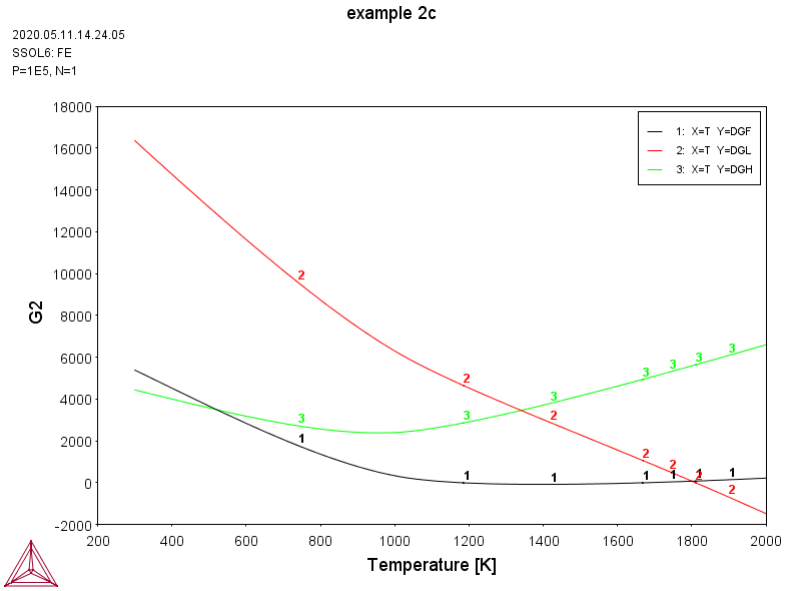
```
POLY: save tcex02a y
   ... the command in full is SAVE_WORKSPACES
POLY: @@ Step along the axis
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
 No initial equilibrium, using default
 Step will start from axis value    300.000
...OK

 Phase Region from    300.000     for:
     BCC_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  1.66747E+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
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex02\tcex02a.POLY3
POLY: @@ Post processing (plotting) is the essential part of this example
POLY: @@ We will plot Gm, Hm and Cp for some phases
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST:
POST: @@ The  x-axis is the temperature in Kelvin
POST: s-d-a x
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
 FILE SYSTEM ERROR IN FILHLP
 ERROR                   1717  READING HELP FILE
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_a2) gm(fcc_a1) gm(liq) gm(hcp_a3)
&
POST:
POST: @@ The table is set as the y-axis and all columns are included
POST: s-d-a y g1
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



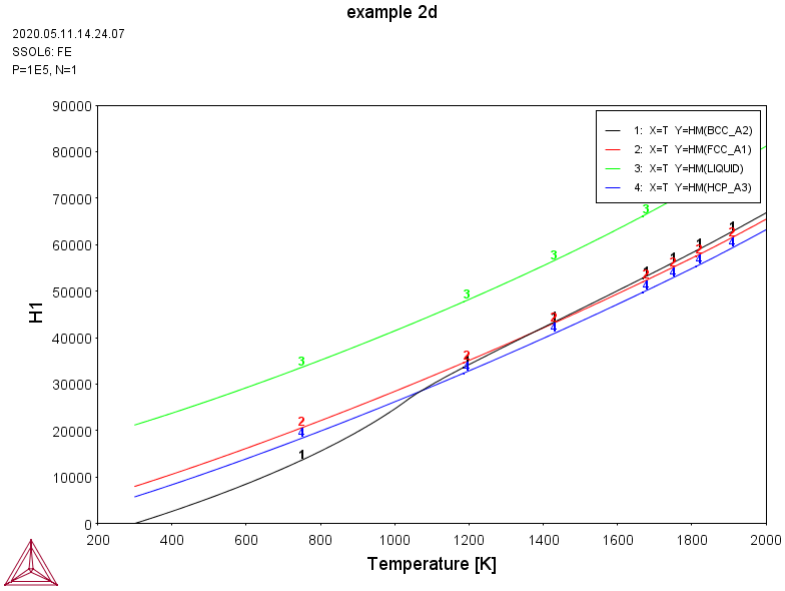

```
POST:
POST:Hit RETURN to continue
POST: @@
POST:
POST:
POST: @@ The magnitude makes it difficult to see anything. Enter
POST: @@ functions for the differences with respect to bcc
POST: ent fun dgf=gm(fcc_a1)-gm(bcc_a2);
   ... the command in full is ENTER_SYMBOL
POST: ent fun dgl=gm(liq)-gm(bcc_a2);
   ... the command in full is ENTER_SYMBOL
POST: ent fun dgh=gm(hcp_a3)-gm(bcc_a2);
   ... the command in full is ENTER_SYMBOL
POST: @@ and enter a new table and set it as the y-axis
POST: ent tab g2
   ... the command in full is ENTER_SYMBOL
Variable(s): dgf dgl dgh;
POST: s-d-a y g2
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ In order to have some identification on the lines
POST: @@ use the command Set_Label
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: D
POST: set-title example 2c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

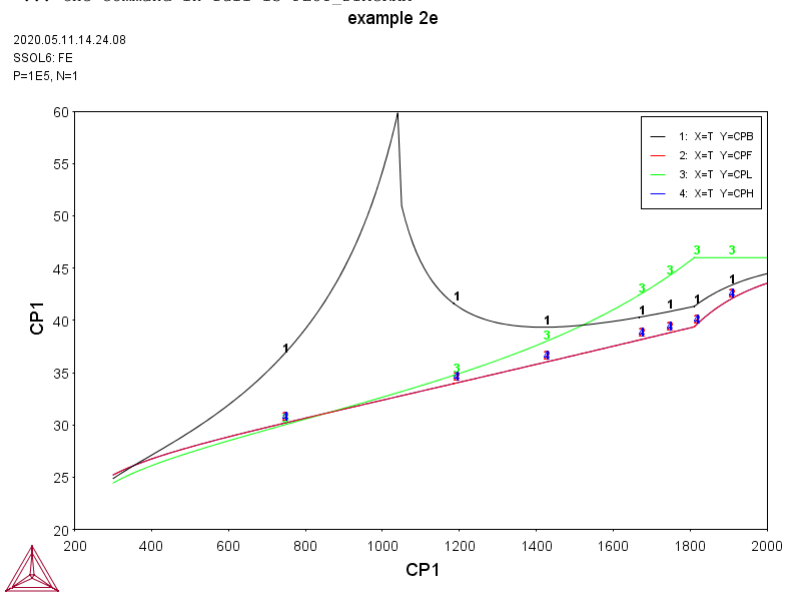



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot enthalpies
POST: ent tab h1
   ... the command in full is ENTER_SYMBOL
Variable(s): hm(bcc_a2) hm(fcc_a1) hm(liq) hm(hcp_a3);
POST: s-d-a y h1
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



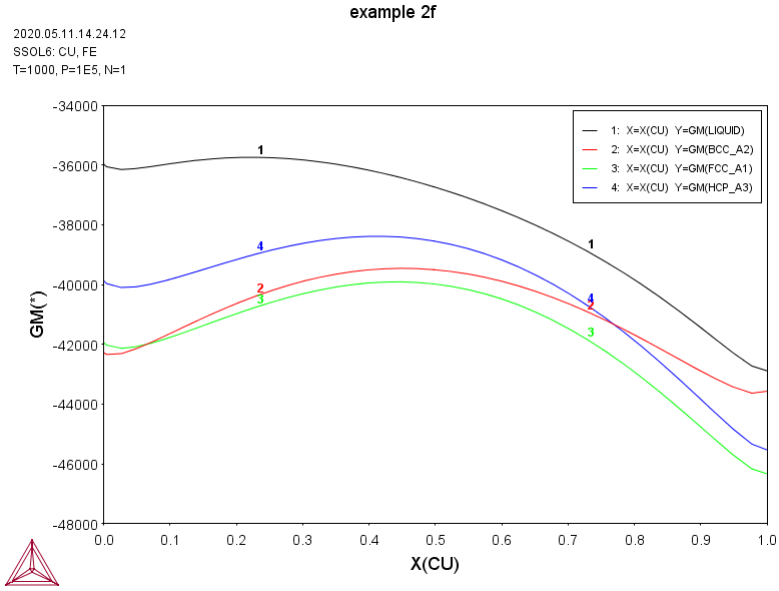

```
POST:
POST:Hit RETURN to continue
POST: @@ And finally plot heat capacities
POST: ent fun cpb=hm(bcc_a2).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cpf=hm(fcc_a1).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cpl=hm(liq).t;
   ... the command in full is ENTER_SYMBOL
POST: ent fun cph=hm(hcp_a3).t;
   ... the command in full is ENTER_SYMBOL
POST: ent tab cp1
   ... the command in full is ENTER_SYMBOL
Variable(s): t cpb cpf cpl cph;
POST: s-d-a y
   ... the command in full is SET_DIAGRAM_AXIS
VARIABLE : cp1
COLUMN NUMBER /*/: 2-5
POST: s-d-a x cp1 1
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 2e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
```

```
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

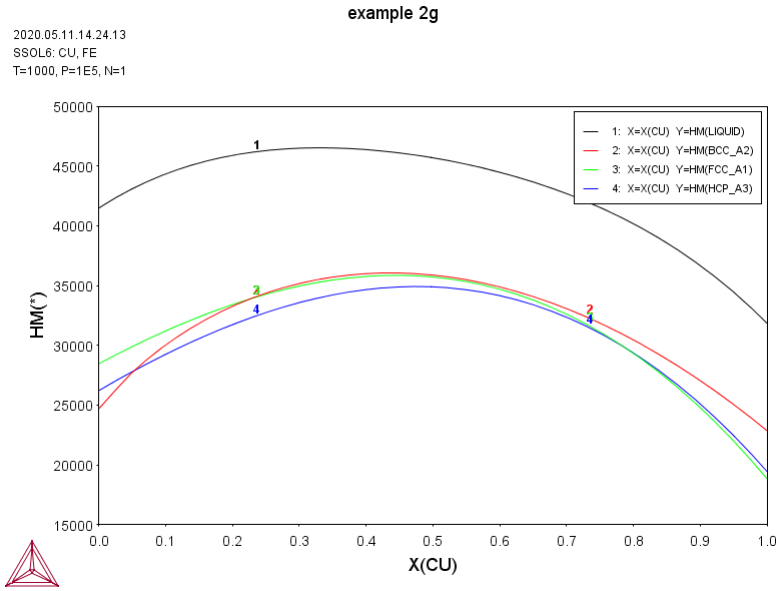



```
POST:
POST:Hit RETURN to continue
POST:
POST: @@ The next example plots functions for a binary system
POST:
POST: ba
   ... the command in full is BACK
POLY: go da
   ... the command in full is GOTO_MODULE
TDB_SSOL6: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 BCC_B2                  FCC_L12                 FCC_COV
 FCC_AUCU                HCP_ORD  REJECTED
 GAS:G  REJECTED
 REINITIATING GES .....
TDB_SSOL6: @@ Select the Cu-Fe system and only
TDB_SSOL6: @@ the fcc, bcc, liquid and hcp phases
TDB_SSOL6: d-sys fe cu
   ... the command in full is DEFINE_SYSTEM
 FE                      CU  DEFINED
TDB_SSOL6: rej ph /all
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  HCP_ZN                  TETRAGONAL_U
 CBCC_A12                CUB_A13                 ORTHORHOMBIC_A20
 LAVES_C14               LAVES_C15               LAVES_C36
 M4N                     ALCU_ETA                ALCU_EPSILON
 ALCUZN_GAMMA_H          AL5FE4                  CUPD_B2
 CUTI                    CU4TI                   CU6Y
 CUZN_GAMMA              D_GAMMA                 FEPD
 FEPD3                   FESB                    FEU6
 FE2U                    FEUZR_DELTA             FEZR2
 FEZR3  REJECTED
TDB_SSOL6: rest ph fcc_a1 bcc_a2 liq hcp_a3
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  LIQUID:L
 HCP_A3  RESTORED
TDB_SSOL6: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 LIQUID:L    :CU FE:
 FCC_A1      :CU FE:VA:
 BCC_A2      :CU FE:VA:
 HCP_A3      :CU FE:VA:
TDB_SSOL6: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Data for the Cu-Fe system are from an unpublished assessment of I Ansara
      and A Jansson published in the COST507 final report: COST507
      Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,
       AT Dinsdale and MH Rand, July 1998, EUR18499. The data were also
      reported by A Jansson in the KTH report TRITA-MAC-533, 1993. >> Cu-Fe '
 -OK-
TDB_SSOL6: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ Set conditions for a single equilibrium
POLY: s-c t=1000,p=1e5,n=1,w(cu)=.01
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           836 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: @@ Select the fraction of Cu as the axis variable
```

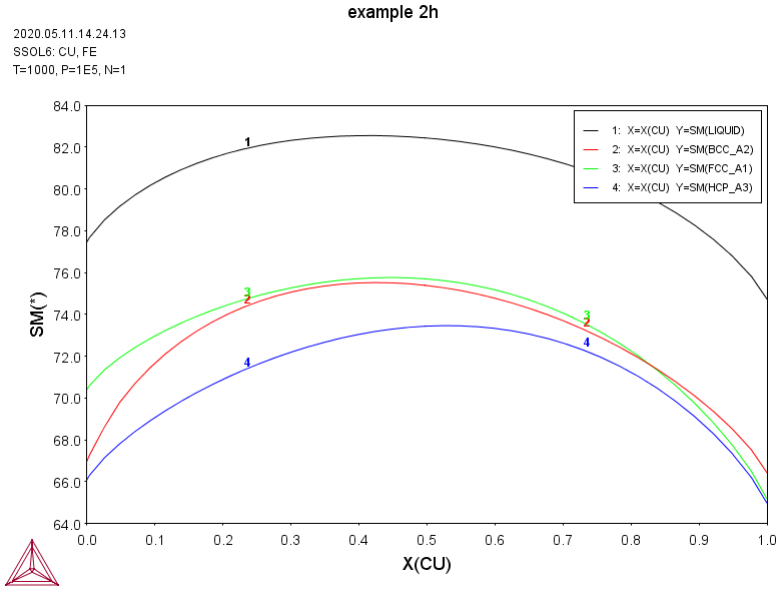
```
POLY: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(cu)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY: @@ Remember to Save
POLY: save tcex02b y
   ... the command in full is SAVE_WORKSPACES
POLY: @@ Now a special STEP option is selected because the NORMAL
POLY: @@ option only calculates the stable phases. The option
POLY: @@ SEPARATE means that all entered phases are calculated
POLY: @@ separately.
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: ?
 The following options are available:
 NORMAL             Stepping with given conditions
 INITIAL_EQUILIBRIA An initial equilibrium stored at every step
 EVALUATE           Specified variables evaluated after each step
 SEPARATE_PHASES    Each phase calculated separately
 T-ZERO             T0 line calculation
 PARAEQUILIBRIUM    Paraequilibrium diagram
 MIXED_SCHEIL       Scheil with fast diffusing elements
 ONE_PHASE_AT_TIME  One phase at a time
Option? /NORMAL/: sep

 Phase Region from   0.529789     for:
     LIQUID
     BCC_A2
     FCC_A1
     HCP_A3

 Phase Region from   0.529789     for:
     LIQUID
     BCC_A2
     FCC_A1
     HCP_A3
 *** Buffer saved on file *** c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex02\tcex02b.POLY3
POLY: @@ Now plot the results in various ways
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: @@ Set the Gm of all phases on the y-axis
POST: s-d-a y gm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: @@ and the mole percent of Cu on the x-axis
POST: s-d-a x x(cu)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 2f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot the enthalpy
POST: s-d-a y hm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2g
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



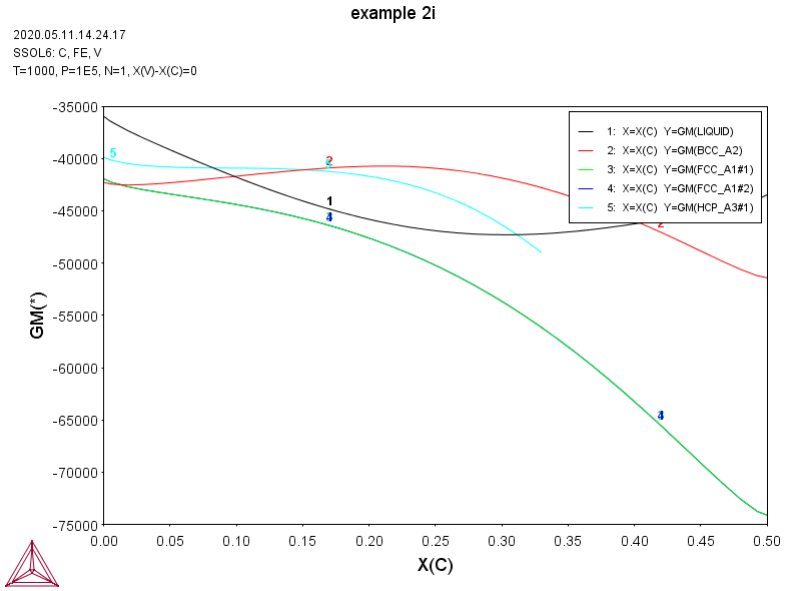

```
POST:
POST:Hit RETURN to continue
POST: @@ and finally the entropy
POST: s-d-a y sm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ The last example plots the Fe-V-C ternary system.
POST: @@ Calculate and plot Gm from the iron corner to VC
POST: ba
   ... the command in full is BACK
POLY: go da
   ... the command in full is GOTO_MODULE
TDB_SSOL6: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 BCC_B2                  FCC_L12                 FCC_COV
 FCC_AUCU                HCP_ORD  REJECTED
 GAS:G  REJECTED
 REINITIATING GES .....
TDB_SSOL6: d-sys fe v c
   ... the command in full is DEFINE_SYSTEM
 FE                      V                       C
   DEFINED
TDB_SSOL6: rej ph / all
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 TETRAGONAL_U            CBCC_A12                CUB_A13
 ORTHORHOMBIC_A20        SIGMA                   GRAPHITE
 LAVES_C14               LAVES_C15               LAVES_C36
 CEMENTITE               KSI_CARBIDE             M23C6
 M7C3                    M3C2                    V3C2
 M5C2                    MC_ETA                  M4N
 FECN_CHI                ALM_D019                AL5FE4
 ALTA_SIGMA              ALTI                    FEPD
 FEPD3                   FESB                    FEU6
```

```
 FE2U                    FEUZR_DELTA             FEZR2
 FEZR3                   V3SI  REJECTED
TDB_SSOL6: rest ph fcc_a1 bcc_a2 hcp_a3 liq
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  HCP_A3
 LIQUID:L  RESTORED
TDB_SSOL6: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set HCP_A3#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Data for the C-Fe system are taken from the assessment of P Gustafson,
      Report TRITA-MAC-0237, October 1984, Scand. J. Metall., 1985, 14, 259
      -267. "A Thermodynamic Evaluation of the Fe-C system". Data for other
      phases not stable in the binary system are from: WM Huang: Report
      TRITA-MAC 411 (Rev 1989); Metall. Trans. A, 1990, 21A, 2115-2123. "A
      Thermodynamic Assessment of the Fe-Mn-C system", WM Huang: Report
      TRITA-MAC 441 (1990), Metall. Trans. A, 1991, 22A(9), 1911-1920. "
      Thermodynamic Properties of the Fe-Mn-V-C System", BJ Lee (1991),
      unpublished revision of data for the C-Cr-Fe-Ni system. H Du and M
      Hillert: Z. Metallkde, 1991, 82(4), 310-316. "An Assessment of the Fe
      -C-N System". H Du: J. Phase Equil., 1993, 14(6), 682-693. "A
      Reevaluation of the Fe-N and Fe-C-N systems". Note: Data for the V3C2
      phase were modified to be 10 J/mol more positive than those for the
      M3C2 phase. The data for the liquid data were modified by Tatjana
      Buhler to prevent bcc phase from becoming stable at high temperatures.
      >> C-Fe '
  'P. Franke, unpublished revisions, Aachen, 2006-2008'
  'Data for the C-Fe-V system are taken the assessments of WM Huang: Report
      TRITA-MAC 432 (1990), Z. Metallkde, 1991, 82(5), 391-401. "A
      thermodynamic evaluation of the Fe-V-C system". BJ Lee and DN Lee:
      Report TRITA-MAC 474 (1991), Calphad, 1991, 15(3), 293-306. "A
      thermodynamic study on the Fe-V-C system". >> C-Fe-V '
  'Data for the C-V system are taken from the assessment of WM Huang: Z.
      Metallkde, 1991, 82, (3), 174-181. "An Assessment of the V-C System".
      Additional data are from further work by WM Huang: Report TRITA-MAC
      441 (1990), BJ Lee: Report TRITA-MAC 475 (1991). >> C-V '
  'Data for the Fe-V system are from the assessments of WM Huang: TRITA-MAC
      432 (Rev 1989,1990), Z. Metallkde, 1991, 82(5), 391-401. "A
      thermodynamic evaluation of the Fe-V-C system", WM Huang: Met. Trans.
      A, 1991, 22(9), 1911-1920. "Thermodynamic properties of the Fe-Mn-V-C
      system". >> Fe-V '
 -OK-
TDB_SSOL6: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ Set conditions for a single equilibrium
POLY: s-c t=1000,p=1e5,n=1,w(v)=.0015,x(c)=.001
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          7821 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: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL6

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

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.57951E+01
 Total Gibbs energy -4.23963E+04,  Enthalpy  2.45646E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.0000E-03  2.1527E-04 3.4515E-02 -2.7990E+04 SER
 FE                      9.9736E-01  9.9828E-01 6.1891E-03 -4.2279E+04 SER
 V                       1.6429E-03  1.5000E-03 4.0605E-07 -1.2236E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.9814E-01, Mass 5.5735E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.99368E-01  V   6.07213E-04  C   2.49276E-05

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.8638E-03, Mass 6.0520E-02, Volume fraction 0.0000E+00  Mass fractions:
 V   8.23694E-01  C   1.75507E-01  FE  7.99487E-04
POLY:Hit RETURN to continue
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FCC_A1#2                ENTERED      0.000000E+00    1.863776E-03
 BCC_A2                  ENTERED      0.000000E+00    9.981362E-01
 FCC_A1#1                ENTERED     -3.462152E-02    0.000000E+00
 HCP_A3#2                ENTERED     -2.875358E-01    0.000000E+00
 HCP_A3#1                ENTERED     -2.875358E-01    0.000000E+00
 LIQUID                  ENTERED     -6.510578E-01    0.000000E+00
POLY:Hit RETURN to continue
POLY: @@ Note we have several composition sets because fcc
POLY: @@ (and possibly hcp) can exist both as metallic and
POLY: @@ as carbide. However, in this case it is unnecessary
POLY: @@ as we are only interested in the value of the
POLY: @@ thermodynamic functions, not the equilibrium, and therefore
POLY: @@ we suspend them
POLY:
POLY: c-s p hcp_a3#2
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: sus
```

```
POLY: 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: @@ We would like to calculate the Gibbs energy from
POLY: @@ pure Fe to the corner VC. Select a line with equal
POLY: @@ fraction of V and C
POLY: s-c x(v)-x(c)=0
   ... the command in full is SET_CONDITION
POLY: s-c w(v)=none
   ... the command in full is SET_CONDITION
POLY: 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: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
    14 ITS,  CPU TIME USED   1 SECONDS
POLY: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL6

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

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.57983E+01
 Total Gibbs energy -4.23424E+04,  Enthalpy  2.46245E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.0000E-03  2.1526E-04 9.5381E-02 -1.9538E+04 SER
 FE                      9.9800E-01  9.9887E-01 6.1904E-03 -4.2277E+04 SER
 V                       1.0000E-03  9.1295E-04 1.6021E-07 -1.3010E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.9858E-01, Mass 5.5752E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.99691E-01  V   2.40126E-04  C   6.83917E-05

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.4208E-03, Mass 4.5810E-02, Volume fraction 0.0000E+00  Mass fractions:
 V   8.19759E-01  C   1.78955E-01  FE  1.28625E-03
POLY:Hit RETURN to continue
POLY: @@ Set the fraction of C as the axis
POLY: @@ The fraction of V will be the same
POLY: 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: save tcex02c y
   ... the command in full is SAVE_WORKSPACES
POLY: @@ step along the axis
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: sep

 Phase Region from   0.330065     for:
     LIQUID
     BCC_A2
     FCC_A1#1
     FCC_A1#2

 Phase Region from   0.330065     for:
     LIQUID
     BCC_A2
     FCC_A1#1
     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 *** c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex02\tcex02c.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: @@ plot the Gm versus carbon content
POST: l-p-s
   ... the command in full is LIST_PLOT_SETTINGS
 GRAPHIC DEVICE: TC-UNITE Driver ( #22)  PLOTFILE: SCREEN
 FONT:  (# 1)  Arial Bold
 AXIS PLOT            YES
 RASTER PLOT         : NO
 TRIANGULAR PLOT     : NO

 AUTOMATIC SCALING

 AUTOMATIC AXIS TEXT

 AXIS VARIABLES
POST: s-d-a x x(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y gm(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST:
POST: set-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 2i
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ This example is about more partial derivatives
POST: back
POLY: go da
   ... the command in full is GOTO_MODULE
TDB_SSOL6: rej sys
   ... the command in full is REJECT
 VA  DEFINED
 BCC_B2                  FCC_L12                 FCC_COV
 FCC_AUCU                HCP_ORD  REJECTED
 GAS:G  REJECTED
 REINITIATING GES .....
TDB_SSOL6: def-sys al cu
   ... the command in full is DEFINE_SYSTEM
 AL                      CU  DEFINED
TDB_SSOL6: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 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

  'Taken from ACMSZ-1, based on unpublished assessment of N Saunders
      published in the COST507 final report COST507 Thermochemical database
      for light metal alloys, Volume 2 eds I Ansara, A T Dinsdale and M H
      Rand, July 1998, EUR18499 Updates from V.T. Witusiewicz, U. Hecht,
      S.G. Fries, S. Rex, JALCOM 385 (2004) 133-143 (Al-Cu) and H.Liang,
      Y.A.Chang, JPE 19 (1998) 25-37 (Al-Cu-Zn). >> Al-Cu '
  'C Servant and I Ansara: J. Chim. Phys. 1997, 94, 869-888. "Thermodynamic
      assessment of the Al-Nb system". >> Al-Nb '
  ' F. Yin, X. Su, Z. Li, P. Zhang, Z. Metallkde, 92, 5 (2001) 447-450. Data
      from Thermodata - supplied to SGTE December 2007 >> Al-Pr '
  'SG Fries, HL Lukas, R Konetzki, and R Schmid-Fetzer: J. Phase Equil.,
      1994, 15(6), 606-614. "Experimental investigation and thermodynamic
      optimization of the Y-Cu binary system". Note: The data for the CuY
      phase have been modified slightly to correct the calculated invariant
      temperatures. >> Cu-Y '
  'M Kowalski and PJ Spencer: J. Phase Equil., 1993, 14(4), 432-438. "
      Thermodynamic reevaluation of the Cu-Zn system". Some v. minor
      differences in gamma_brass data wrt SOLDERS >> Cu-Zn '
  'Liang Y, Guo C, Li C, Du Z, Journal of Alloys and Compounds, 2008, 460,
      314-319 "Thermodynamic modeling of the Al-Cr system." >> Al-Cr '
  'Data for the Al-Li system are from an unpublished assessment of N
      Saunders published in the COST507 final report: COST507 Thermochemical
      Database for Light Metal Alloys, Vol 2, eds by I Ansara, AT Dinsdale
      and MH Rand, July 1998, EUR18499. >> Al-Li '
  ' Data supplied by Thermodata to SGTE - December 2007 A. Saccone, G.
      Cacciamani, D. Maccio, G. Borzone, R. Ferro, Intermetallics, 6 (1998)
      201-215. >> Al-Sm '
  'W. Huang, S.M. Opalka, D. Wang, T.B. Flanagan, Calphad, 31, 315-29(2007) >
      > Cu-Pd '
 -OK-
TDB_SSOL6: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: s-c t=1400 p=1e5 n=1 x(al)=.1
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         11669 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: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL6

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

```
 Temperature   1400.00 K (  1126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.98896E+01
 Total Gibbs energy -8.53069E+04,  Enthalpy  3.62263E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      1.0000E-01  4.5053E-02 1.3593E-06 -1.5724E+05 SER
 CU                      9.0000E-01  9.5495E-01 1.3045E-03 -7.7314E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.9890E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  9.54947E-01  AL  4.50529E-02
POLY:Hit RETURN to continue
POLY: @@ Check the activity of aluminum
POLY: show acr(al)
   ... the command in full is SHOW_VALUE
 ACR(AL)=1.359263E-6
POLY: @@ This activity value is referred to fcc Al at 298.15 K.
POLY: @@ Set the proper reference state for activities
POLY: set-ref-state al
   ... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature /*/:
Pressure /1E5/:
POLY:
POLY: set-ref-state cu
   ... the command in full is SET_REFERENCE_STATE
Reference phase: liq
Temperature /*/:
Pressure /1E5/:
POLY:
POLY: show acr(al)
   ... the command in full is SHOW_VALUE
 ACR(AL)=8.0990275E-4
POLY: @@ This value is better. The corresponding chemical potential is
POLY: show mur(al)
   ... the command in full is SHOW_VALUE
 MUR(AL)=-82862.697
POLY: @@ The relation is simply that acr(al)=exp(mur(al)/RT). Check that
POLY: enter fun test
   ... the command in full is ENTER_SYMBOL
Function: exp(mur(al)/8.31451/T);
POLY: show test
   ... the command in full is SHOW_VALUE
 TEST=8.0990275E-4
POLY:Hit RETURN to continue
POLY: @@ POLY allows the calculation of partial derivatives of thermodynamic
POLY: @@ quantities of original reference state with respect to fractions
POLY: @@ that are conditions. For example
POLY: show gm.x(al)
   ... the command in full is SHOW_VALUE
 GM.X(AL)=-79930.097
POLY: @@ This is not the same as the chemical potential. It actually
POLY: @@ is equal to the so-called diffusion potential: mu(al)-mu(cu).
POLY:
POLY: ent fun diffmu=mu(al)-mu(cu);
   ... the command in full is ENTER_SYMBOL
POLY: show diffmu
   ... the command in full is SHOW_VALUE
 DIFFMU=-79930.097
POLY: @@ The relation between the chemical potential and the partial derivative is
POLY: @@ mu(al) = gm + gm.x(al) - x(al)*gm.x(al)
POLY:
POLY: @@ We can also enter this as a function.
POLY: enter fun dgdx=gm+gm.x(al)-x(al)*gm.x(al);
   ... the command in full is ENTER_SYMBOL
POLY: sh dgdx
   ... the command in full is SHOW_VALUE
 DGDX=-157243.97
POLY: sh mu(al)
   ... the command in full is SHOW_VALUE
 MU(AL)=-157243.97
POLY: @@ Partial entropy is the negative of mu(al).t
POLY: ent fun ps=-mu(al).t;
   ... the command in full is ENTER_SYMBOL
POLY: sh ps
   ... the command in full is SHOW_VALUE
 PS=95.218667
POLY: @@ Partial enthalpy is h = g + s*t
POLY: enter fun ph=mu(al)+ps*t;
   ... the command in full is ENTER_SYMBOL
POLY: sh ph
   ... the command in full is SHOW_VALUE
 PH=-23937.838
POLY: @@ Partial enthalpy can also be calculated in a similar way as chemical
POLY: @@ potential
POLY: @@ partial enthalpy = hm + hm.x(al) - x(al)*hm.x(al)
POLY: ent fun ph1=hm+hm.x(al)-x(al)*hm.x(al);
   ... the command in full is ENTER_SYMBOL
POLY: sh ph1
   ... the command in full is SHOW_VALUE
 PH1=-23937.838
POLY: @@ As can be seen, ph1 = ph.
POLY: @@ Another useful quantity is mu(al).x(al).  That is related to
POLY: @@ the thermodynamic factor and part of the diffusion coefficient.
POLY: show mu(al).x(al)
   ... the command in full is SHOW_VALUE
 MU(AL).X(AL)=324789.82
POLY:
POLY: set-inter
   ... the command in full is SET_INTERACTIVE
POLY:
```

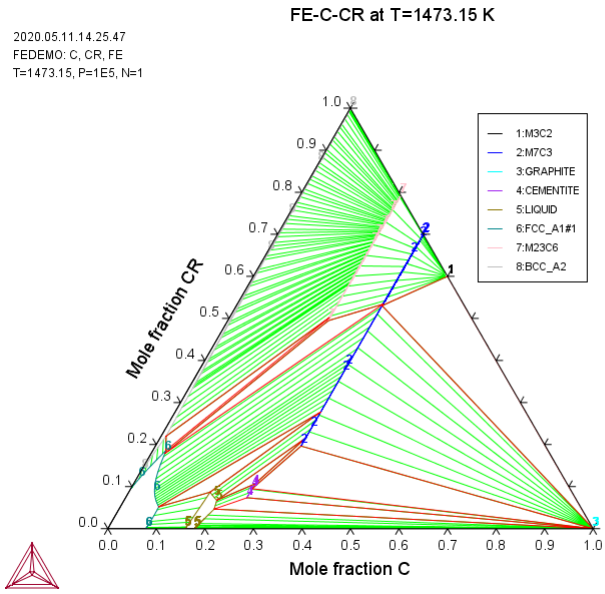
tcex03

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex03\tcex03.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating an isothermal section using the 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
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
 Current database: Iron Demo Database v3.0

 VA                      /-  DEFINED
Database: /FEDEMO/: FEDEMO
First element: ?
 No list of assessed systems in this database
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/: Y
 VA                      /-  DEFINED
 REINITIATING GES .....
 C                       CR                      FE
   DEFINED

 ***********************************************************
 * WARNING: This database has no list of assessed systems *
 *            The diagram may be wrong.                   *
 ***********************************************************

Quit? /Y/: N
14:25:39,254 INFO  *** Invoking Gibbs Energy System v6 ***
 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
 Creating a new composition set FCC_A1#2
   ... 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) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
  'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C -Cr-Nb'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
      -C'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  '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'
  'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.J. Lee, unpublished work at KTH (1999); update of steel database'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
  'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
      TCFE9 database (TCFE v9.0, Jan, 2017).'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'P. Villars, L.D. Calvert. Pearsons handbook of crystallographic data for
      intermetallic phases, Metals park, Ohio 1985: American society for
      metals'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
       CR-FE-MO'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992)
```

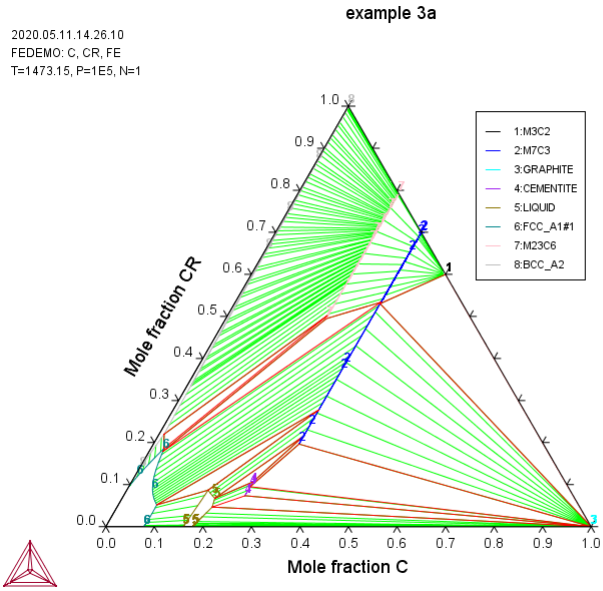
```
     Revision; C-Cr-Fe-Mo'
 'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C -FE-MO'
 'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
     (1987); C-CR-FE-W'
 'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
     -FE-N'
 'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
     (2011) 479-491; Fe-Mn-C'
 'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
     Sigma model'
-OK-
The condition X(CR)=.1234  created
The condition X(FE)=.1234  created

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
Generating start equilibrium  1
Generating start equilibrium  2
Generating start equilibrium  3
Generating start equilibrium  4
Generating start equilibrium  5
Generating start equilibrium  6
Generating start equilibrium  7
Generating start equilibrium  8
Generating start equilibrium  9

Organizing start points

Using ADDED start equilibria

Generating start point   1
Generating start point   2
Generating start point   3
Generating start point   4
Generating start point   5
Generating start point   6
Generating start point   7
Generating start point   8
Generating start point   9
Generating start point  10
Working hard
Generating start point  11
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Generating start point  21

Phase region boundary   1 at:   1.750E-01  1.750E-01
 ** GRAPHITE
    M7C3
Calculated.                     11 equilibria

Phase region boundary   2 at:   2.652E-01  8.482E-02
 ** GRAPHITE
 ** M3C2
    M7C3

Phase region boundary   3 at:   5.652E-01  8.482E-02
 ** M3C2
    M7C3
Calculated                     20 equilibria

Phase region boundary   4 at:   3.000E-01  0.000E+00
    GRAPHITE
 ** M3C2

Phase region boundary   5 at:   2.652E-01  8.482E-02
 ** GRAPHITE
    M7C3
Calculated.                     18 equilibria

Phase region boundary   6 at:   9.822E-02  2.518E-01
 ** CEMENTITE
 ** GRAPHITE
    M7C3

Phase region boundary   7 at:   1.457E-01  5.793E-01
 ** CEMENTITE
    M7C3
Calculated.                      3 equilibria

Phase region boundary   8 at:   1.610E-01  5.640E-01
 ** LIQUID
 ** CEMENTITE
    M7C3

Phase region boundary   9 at:   1.414E-01  6.131E-01
 ** LIQUID
    M7C3
Calculated.                      7 equilibria

Phase region boundary  10 at:   1.820E-01  5.842E-01
 ** LIQUID
 ** FCC_A1#1
    M7C3

Phase region boundary  11 at:   1.646E-01  6.458E-01
 ** FCC_A1#1
    M7C3
Calculated.                     28 equilibria

Phase region boundary  12 at:   3.658E-01  4.629E-01
 ** FCC_A1#1
 ** M23C6
    M7C3

Phase region boundary  13 at:   5.141E-01  2.324E-01
```

```
 ** M23C6
    M7C3
Calculated                      33 equilibria

Phase region boundary  14 at:   3.369E-01  5.455E-01
    FCC_A1#1
 ** M23C6
Calculated.                      2 equilibria

Phase region boundary  15 at:   3.450E-01  5.382E-01
 ** BCC_A2
    FCC_A1#1
 ** M23C6

Phase region boundary  16 at:   2.028E-01  7.787E-01
 ** BCC_A2
    FCC_A1#1
Calculated                      21 equilibria

Phase region boundary  17 at:   3.620E-01  5.294E-01
 ** BCC_A2
    M23C6
Calculated                      65 equilibria

Phase region boundary  18 at:   6.933E-02  8.073E-01
    LIQUID
 ** FCC_A1#1
Calculated                      26 equilibria

Phase region boundary  19 at:   8.694E-02  6.926E-01
 ** LIQUID
    CEMENTITE
Calculated.                      5 equilibria

Phase region boundary  20 at:   6.004E-02  7.169E-01
 ** LIQUID
    CEMENTITE
 ** GRAPHITE

Phase region boundary  21 at:   3.674E-02  3.383E-01
    CEMENTITE
 ** GRAPHITE
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   2.330E-02  3.787E-01
    LIQUID
 ** GRAPHITE
Calculated                      19 equilibria

Phase region boundary  23 at:   1.750E-01  1.750E-01
 ** GRAPHITE
    M7C3
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  24 at:   1.750E-01  1.750E-01
 ** GRAPHITE
    M7C3
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   1.750E-01  1.750E-01
 ** GRAPHITE
    M7C3
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   3.000E-01  0.000E+00
    GRAPHITE
 ** M3C2

Phase region boundary  27 at:   2.652E-01  8.482E-02
 ** GRAPHITE
    M7C3
Calculated.                      1 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   5.652E-01  8.482E-02
 ** M3C2
    M7C3
Calculated                      31 equilibria

Phase region boundary  29 at:   6.432E-01  6.818E-03
 ** M3C2
    M7C3
Calculated                      15 equilibria

Phase region boundary  30 at:   6.432E-01  6.818E-03
 ** M3C2
    M7C3
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   8.930E-01  3.418E-03
    BCC_A2
 ** M23C6
Calculated                      12 equilibria

Phase region boundary  32 at:   8.930E-01  3.418E-03
    BCC_A2
 ** M23C6
Calculated.                     54 equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   1.172E-02  3.947E-01
    LIQUID
 ** GRAPHITE
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   1.172E-02  3.947E-01
    LIQUID
 ** GRAPHITE
Calculated                      22 equilibria
```

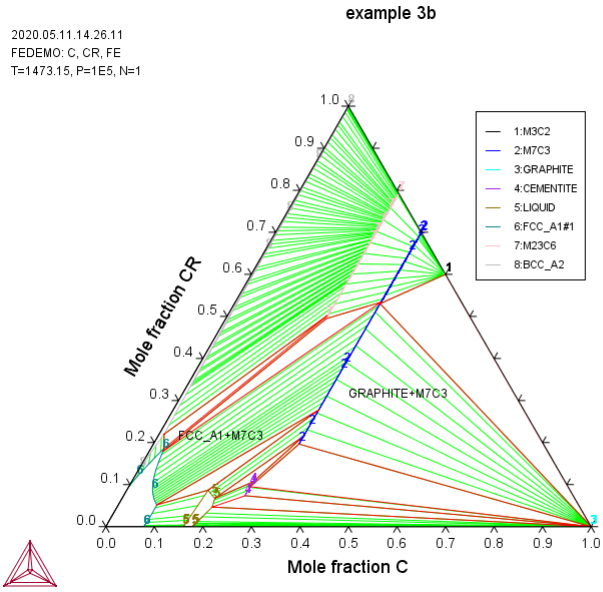
```
 Phase region boundary  35 at:   6.068E-03  4.025E-01
     LIQUID
  ** GRAPHITE
 Calculated.                      4 equilibria
 Terminating at known equilibrium

 Phase region boundary  36 at:   6.068E-03  4.025E-01
     LIQUID
  ** GRAPHITE
 Calculated                       9 equilibria

 Phase region boundary  37 at:   1.262E-02  8.673E-01
  ** LIQUID
     FCC_A1#1
 Calculated                      10 equilibria

 Phase region boundary  38 at:   1.262E-02  8.673E-01
  ** LIQUID
     FCC_A1#1
 Calculated.                      7 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   4.578E-01  4.348E-01
     BCC_A2
  ** M23C6
 Calculated                      57 equilibria

 Phase region boundary  40 at:   4.578E-01  4.348E-01
     BCC_A2
  ** M23C6
 Calculated.                      11 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   6.789E-01  2.163E-01
     BCC_A2
  ** M23C6
 Calculated                      30 equilibria

 Phase region boundary  42 at:   6.789E-01  2.163E-01
     BCC_A2
  ** M23C6
 Calculated.                      33 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\ISOTHER_002.POLY3
 CPU time for mapping                     7 seconds
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes
```




```
POST:
POST: set-title example 3a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

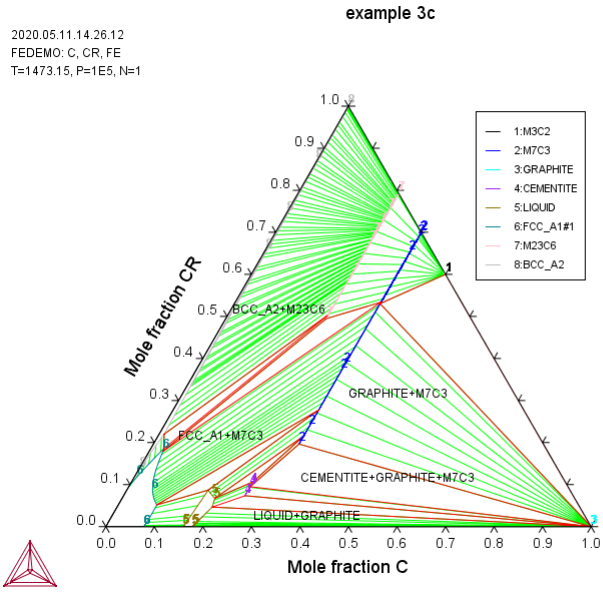



```
POST:
POST:Hit RETURN to continue
POST: @@ Add some labels
POST: add .35 .3
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: GRAPHITE+M7C3
Text size: /.36/:
POST: add .05 .2
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: FCC_A1+M7C3
Text size: /.36/:
POST: set-title example 3b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

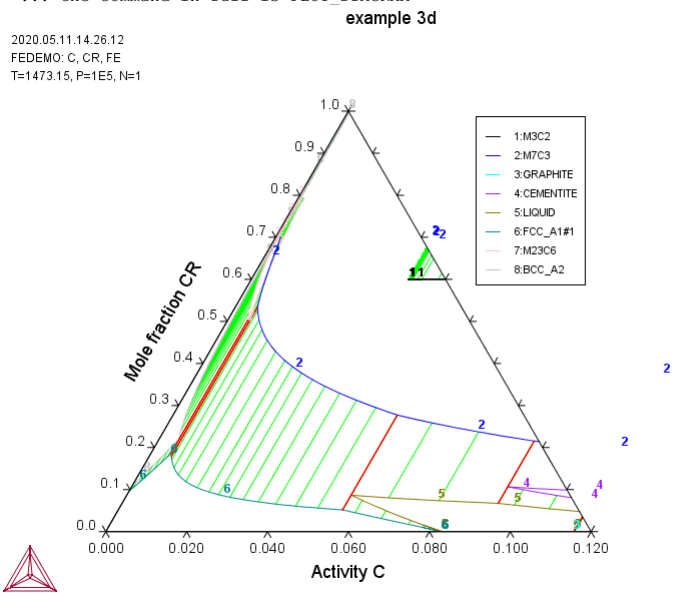



```
POST:
POST:Hit RETURN to continue
POST: add .3 .01
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: LIQUID+GRAPHITE
Text size: /.36/:
POST: add .35 .1
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
```

```
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: CEMENTITE+GRAPHITE+M7C3
Text size: /.36/:
POST: add .01 .5
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_A2+M23C6
Text size: /.36/:
POST: set-title example 3c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

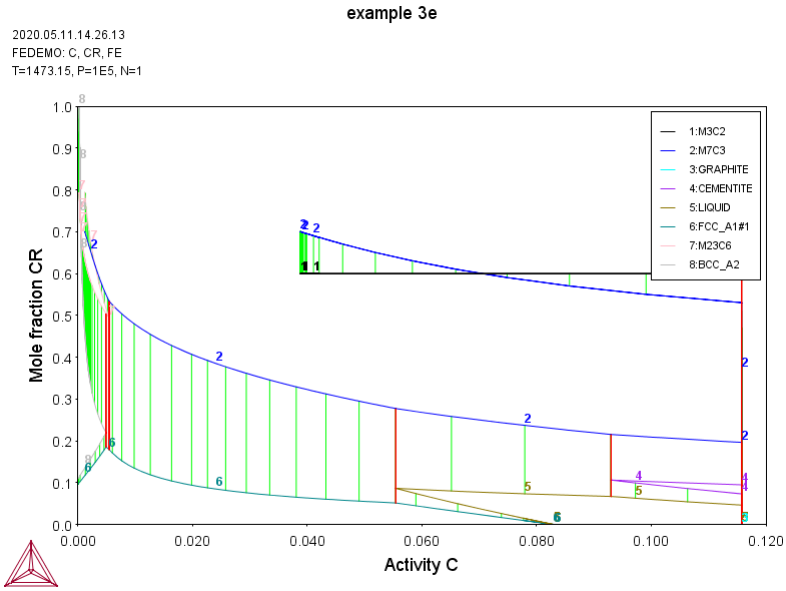



```
POST:
POST:Hit RETURN to continue
POST: @@ We can try the same exercise as in TCEX_01 which uses
POST: @@ carbon activity on one axis
POST: s-d-a x ac c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 3d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

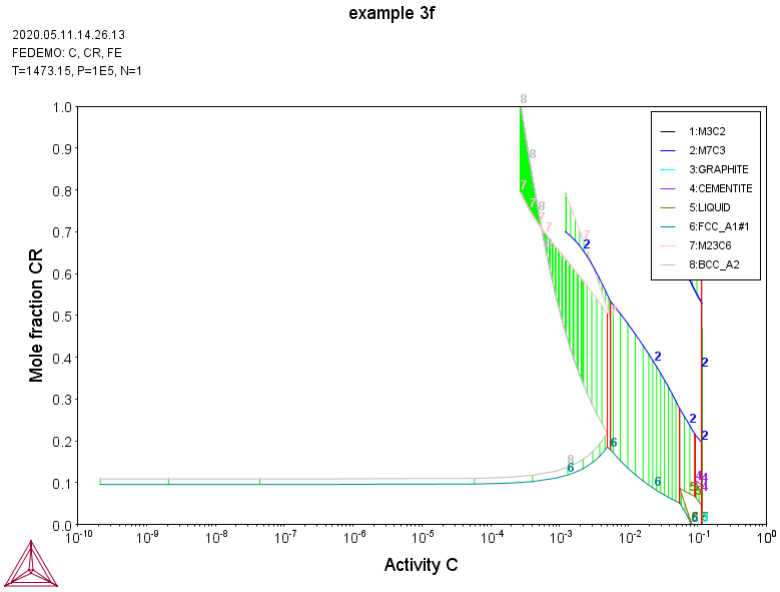



```
POST:
POST:Hit RETURN to continue
POST: @@ With these axes it is better to have a square diagram.
POST: s-dia-type
   ... the command in full is SET_DIAGRAM_TYPE
```

```
TRIANGULAR DIAGRAM  (Y OR N) /N/: N
CREATE TETRAHEDRON WRML FILE  (Y OR N) /N/:
POST:
POST: set-title example 3e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

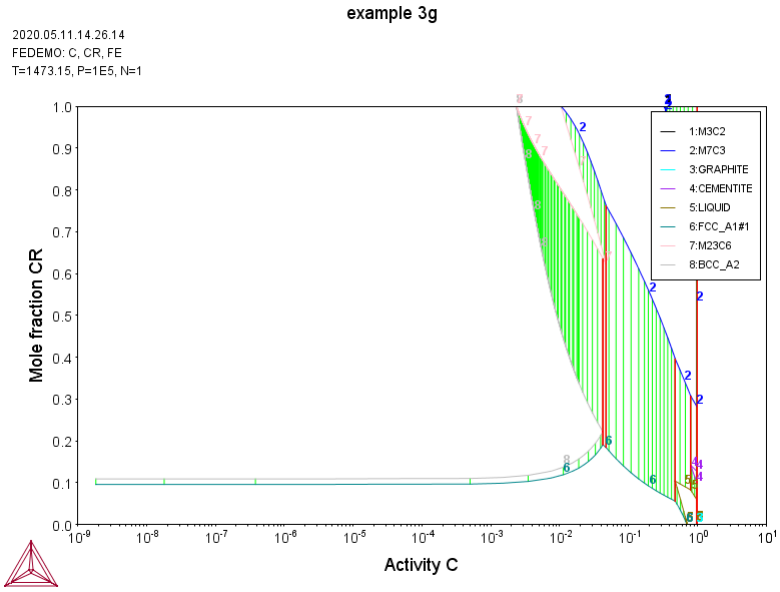



```
POST:
POST:Hit RETURN to continue
POST: @@ The activity axis is probably better as logarithmic
POST: s-a-ty x
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 3f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

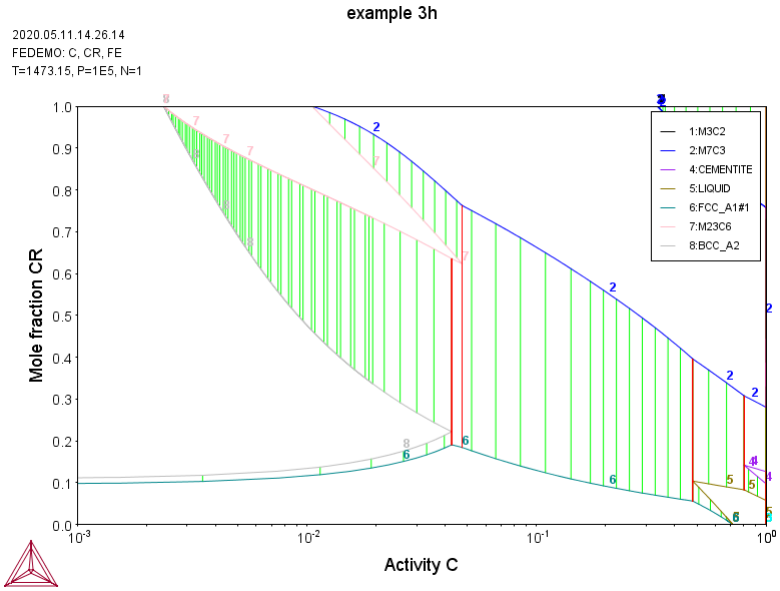



```
POST:
POST:Hit RETURN to continue
POST: @@ In order for pure graphite to have activity one, the reference
POST: @@ state of C should be set to graphite. In addition,
POST: @@ the solubility lines now cross. Is the diagram wrong?
POST: @@ No, in this case one should not use the mole fraction of Cr
POST: @@ but the metallic fraction. This can be fixed by setting
POST: @@ the status of C to "special". All species set as special
POST: @@ are 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:
POLY: s-r-s
   ... the command in full is SET_REFERENCE_STATE
Component: c
```

```
Reference phase: gra
Temperature /*/:
Pressure /1E5/:
POLY: ch-st
   ... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/: c
Name(s): c
Status: /ENTERED/: ?
 FILE SYSTEM ERROR IN FILHLP
 ERROR                 1717  READING HELP FILE
Status: /ENTERED/: special
POLY:
POLY: post
POST:
POST: set-title example 3g
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

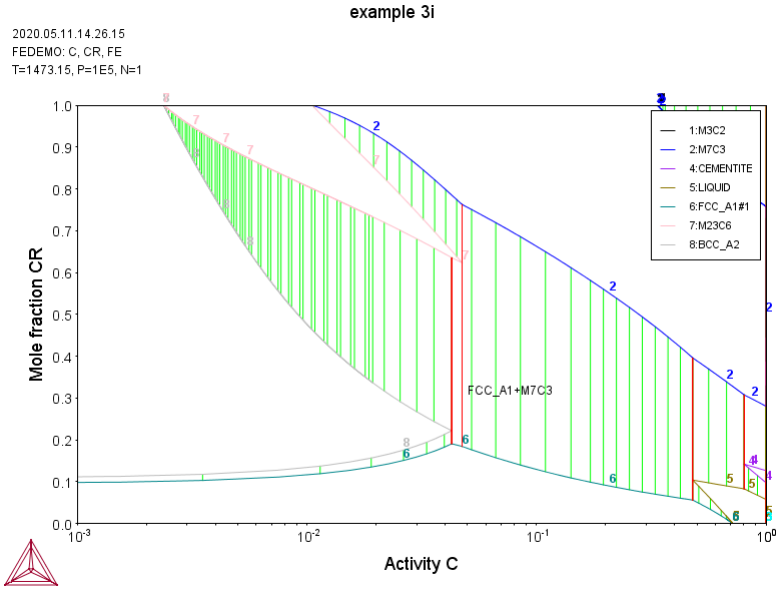



```
POST:
POST:Hit RETURN to continue
POST: @@ Finally scale
POST: s-s x n .001 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 3h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ This kind of diagram is useful to understand diffusion paths.
POST:
POST: @@ The phase labels were lost when we changed axis
POST: @@ To add them back
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
 Stable phases are: FCC_A1+M7C3
Text size: /.36/:
POST: set-title example 3i
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

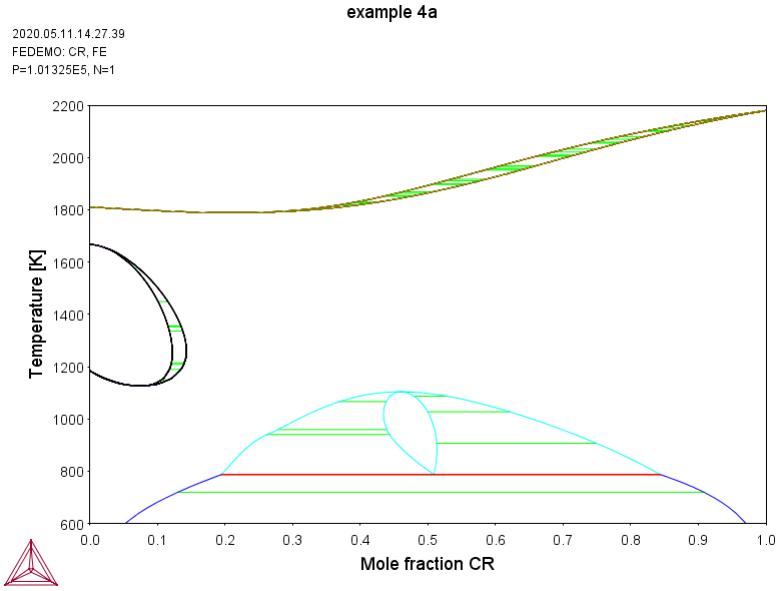
tcex04

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex04\tcex04.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating the miscibility gap in the Fe-Cr system.
SYS:
SYS: set-log ex04,,,
SYS:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw FEDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database v3.0

 VA                      /-  DEFINED
TDB_FEDEMO: def-sys
   ... the command in full is DEFINE_SYSTEM
ELEMENTS: fe cr
 FE                      CR  DEFINED
TDB_FEDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 LIQUID:L    :CR FE:
 BCC_A2      :CR FE:VA:
 LAVES_PHASE_C14 :CR FE:CR FE:
 CBCC_A12    :CR FE:VA:
 CHI_A12     :CR FE:CR:CR FE:
 CUB_A13     :CR FE:VA:
 FCC_A1      :CR FE:VA:
 HCP_A3      :CR FE:VA:
 SIGMA       :CR FE:CR:CR FE:
TDB_FEDEMO: rej ph /all
   ... the command in full is REJECT
 LIQUID:L                BCC_A2                  LAVES_PHASE_C14
 CBCC_A12                CHI_A12                 CUB_A13
 FCC_A1                  HCP_A3                  SIGMA
   REJECTED
TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 sigma
   ... the command in full is RESTORE
 LIQUID:L                FCC_A1                  BCC_A2
 SIGMA  RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
14:27:33,060 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 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) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019'
  'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
  'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
TDB_FEDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 SIGMA                   ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                  ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                  ENTERED      0.000000E+00    0.000000E+00
 LIQUID                  ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CR ENTERED    FE ENTERED    VA ENTERED
POLY:Hit RETURN to continue
POLY: @@ There is a miscibility gap in BCC Fe-Cr.

POLY: @@ Let us first calculate the low temperature region.
```

```
POLY: s-c x(cr)=.6 t=700 p=101325 n=1
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          2579 grid points in             1 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     1  s
 Creating a new composition set BCC_A2#3
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: FEDEMO

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

 Temperature    700.00 K (   426.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.35364E+01
 Total Gibbs energy -2.30658E+04,  Enthalpy  1.31801E+04,  Volume  7.26548E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      6.0000E-01  5.8274E-01 2.3703E-02 -2.1780E+04 SER
 FE                      4.0000E-01  4.1726E-01 1.3643E-02 -2.4995E+04 SER

 BCC_A2#3                    Status ENTERED     Driving force  0.0000E+00
 Moles 6.0116E-01, Mass 3.1437E+01, Volume fraction 6.0322E-01  Mass fractions:
 CR  9.17514E-01  FE  8.24857E-02

 BCC_A2#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 3.9884E-01, Mass 2.2100E+01, Volume fraction 3.9678E-01  Mass fractions:
 FE  8.93487E-01  CR  1.06513E-01
POLY:Hit RETURN to continue
POLY: @@ Now make a calculation at a higher temperature
POLY: s-c t=900
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          2579 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: FEDEMO

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

 Temperature    900.00 K (   626.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.35364E+01
 Total Gibbs energy -3.49346E+04,  Enthalpy  2.36851E+04,  Volume  7.26372E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      6.0000E-01  5.8274E-01 1.2779E-02 -3.2626E+04 SER
 FE                      4.0000E-01  4.1726E-01 5.9087E-03 -3.8398E+04 SER

 SIGMA                       Status ENTERED     Driving force  0.0000E+00
 Moles 6.4237E-01, Mass 3.4605E+01, Volume fraction 6.3941E-01  Mass fractions:
 FE  5.04665E-01  CR  4.95335E-01

 BCC_A2#3                    Status ENTERED     Driving force  0.0000E+00
 Moles 3.5763E-01, Mass 1.8932E+01, Volume fraction 3.6059E-01  Mass fractions:
 CR  7.42495E-01  FE  2.57505E-01
POLY:Hit RETURN to continue
POLY: @@ The Fe-Cr phase diagram has three non-connected two-phase regions.
POLY:
POLY: 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: 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: @@ Always use a SAVE command before MAP (or STEP) otherewise unless
POLY: @@ you want to overlay this calculation with an earlier one
POLY: save tcex04 y
   ... the command in full is SAVE_WORKSPACES
POLY: 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
Calculated                     12 equilibria

Phase region boundary   2 at:   1.067E-02  1.169E+03
    BCC_A2#1
 ** FCC_A1
Calculated                     42 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   5 at:   5.192E-01  7.875E+02
    BCC_A2#1
 ** BCC_A2#2
 ** SIGMA

Phase region boundary   6 at:   6.762E-01  7.875E+02
    BCC_A2#1
 ** SIGMA
Calculated..                    53 equilibria
Calculated                     53 equilibria

Phase region boundary   7 at:   6.762E-01  7.875E+02
    BCC_A2#1
 ** SIGMA
Calculated.                     49 equilibria
Terminating at known equilibrium

Phase region boundary   8 at:   5.119E-01  6.100E+02
 ** BCC_A2#1
    BCC_A2#2
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary   9 at:   5.119E-01  6.100E+02
 ** BCC_A2#1
    BCC_A2#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  10 at:   5.119E-01  6.100E+02
 ** BCC_A2#1
    BCC_A2#2
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  11 at:   4.325E-02  1.137E+03
    BCC_A2#1
 ** FCC_A1
Calculated                     49 equilibria

Phase region boundary  12 at:   4.325E-02  1.137E+03
    BCC_A2#1
 ** FCC_A1
Calculated                     14 equilibria

Phase region boundary  13 at:   1.006E-01  1.137E+03
    BCC_A2#1
 ** FCC_A1
Calculated                     25 equilibria

Phase region boundary  14 at:   1.006E-01  1.137E+03
    BCC_A2#1
 ** FCC_A1
Calculated                     34 equilibria

Phase region boundary  15 at:   1.224E-02  1.663E+03
 ** BCC_A2#1
    FCC_A1
Calculated                     43 equilibria

Phase region boundary  16 at:   1.224E-02  1.663E+03
 ** BCC_A2#1
    FCC_A1
Calculated                     12 equilibria

Phase region boundary  17 at:   9.640E-03  1.809E+03
    LIQUID
 ** BCC_A2#1
Calculated                     11 equilibria

Phase region boundary  18 at:   9.640E-03  1.809E+03
    LIQUID
 ** BCC_A2#1
Calculated                     93 equilibria

Phase region boundary  19 at:   3.471E-01  1.807E+03
    LIQUID
```

```
 ** BCC_A2#1
Calculated                      38 equilibria

Phase region boundary  20 at:   3.471E-01  1.807E+03
    LIQUID
 ** BCC_A2#1
Calculated                      64 equilibria

Phase region boundary  21 at:   6.881E-01  2.007E+03
    LIQUID
 ** BCC_A2#1
Calculated                      68 equilibria

Phase region boundary  22 at:   6.881E-01  2.007E+03
    LIQUID
 ** BCC_A2#1
Calculated                      39 equilibria

Phase region boundary  23 at:   9.910E-01  2.176E+03
    LIQUID
 ** BCC_A2#1
Calculated                      90 equilibria

Phase region boundary  24 at:   9.910E-01  2.176E+03
    LIQUID
 ** BCC_A2#1
Calculated                      12 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex04\tcex04.POLY3
CPU time for mapping                     4 seconds
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST: s-t-s 6
   ... the command in full is SET_TIELINE_STATUS
POST: set_title example 4a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex05

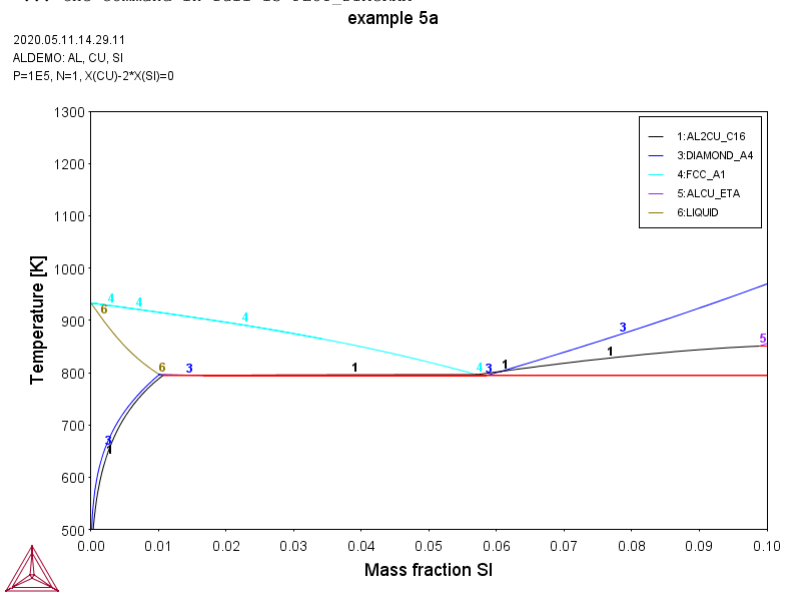
```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex05\tcex05.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a vertical section in the Al-Cu-Si system
SYS:
SYS: @@ This example calculates a vertical section in the Al-Cu-Si
SYS: @@ system and of a vertical section from Al to 10% Cu2Si.
SYS:
SYS: set-log ex05,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw ALDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Aluminum Demo Database v4.0

 VA                      /-  DEFINED
TDB_ALDEMO: def-sys al Cu si
   ... the command in full is DEFINE_SYSTEM
 AL                      CU                      SI
   DEFINED
TDB_ALDEMO: get
   ... the command in full is GET_DATA
14:28:56,742 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, Calphad,15 317-425 (1991)'
  'Volume data from TCFE4, 2006'
  'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
      thermal conductivity'
  'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
  'M Ghasemi, Thermo-Calc Software AB (2020)'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
  'M J Assael, J Phys Chem Ref Data 41 (2012) 033101; Cd, Co, Ga, In, Hg, Si,
       Tl, Zn'
  'I. Ansara (Editor), COST 507, (1998)'
  'M Ghasemi, Thermo-Calc Software AB (2019)'
  'C.-Y. He,Calphad, 33,200-210 (2009),Al-Cu-Si'
  'J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'
  'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),CU-Si'
  'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
      parameter, linear combination of unary volume data'
  'H-L Chen, in TCAL3.0, Assessment, extrapolation and assumption'
  'Hai-Lin Chen, electrical resistivity
       thermal conductivity (2020)'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
  'H-L Chen, Evaluation of molar volume'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
  'Nathalie Dupin, in TCNI6.0, Refinement of Al-Ni'
  'Volume data, N. Dupin 2008'
  'H-L Chen, in TCAL2.0, Assessment, extrapolation and assumption'
  'J.R.Zhao, Y.Du, to be submitted, 2010,Sn-Sr,Cu-Mg-Si'
  'W.H. Sun, unpublished (2010),Cu-Si-Zn,Cu-Ni-Zn'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'H-L Chen, in TCAL1.2, assessment of Al-Cu-Mg-Si'
 -OK-
TDB_ALDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: s-c t=1000,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY: @@ We shall calculate along a line where the Cu content is twice

POLY: @@ that of the Si content. This can be used as a condition.
POLY: @@ Note that the whole equation must be given before the equal sign.
POLY: @@ It is wrong to write s-c x(cu)=2*x(si).
POLY: s-c x(cu)-2*x(si)=0
   ... the command in full is SET_CONDITION
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=1000, P=1E5, N=1, X(CU)-2*X(SI)=0
 DEGREES OF FREEDOM 1
POLY: s-c w(si)=0.05
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
```

```
 Testing POLY result by global minimization procedure
Calculated         17676 grid points in             1 s
    38 ITS,  CPU TIME USED   2 SECONDS
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: ALDEMO

 Conditions:
 T=1000, P=1E5, N=1, X(CU)-2*X(SI)=0, W(SI)=5E-2
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  3.10908E+01
 Total Gibbs energy -5.01533E+04,  Enthalpy  2.90243E+04,  Volume  1.09629E-05

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                       8.3395E-01  7.2374E-01 4.7926E-03 -4.4405E+04 SER
 CU                       1.1070E-01  2.2626E-01 9.6970E-06 -9.5980E+04 SER
 SI                       5.5351E-02  5.0000E-02 4.4065E-03 -4.5103E+04 SER

 LIQUID                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.1091E+01, Volume fraction 1.0000E+00  Mass fractions:
 AL  7.23737E-01  CU  2.26263E-01  SI  5.00000E-02
POLY:@?<Hit_return_to_continue>
POLY: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  GOTO_MODULE              REINITIATE_MODULE
 ADVANCED_OPTIONS         HELP                     SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  INFORMATION              SELECT_EQUILIBRIUM
 BACK                     LIST_AXIS_VARIABLE       SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_CONDITIONS          SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_EQUILIBRIUM         SET_CONDITION
 COMPUTE_TRANSITION       LIST_INITIAL_EQUILIBRIA  SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_STATUS              SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_SYMBOLS             SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
 DEFINE_MATERIAL          MACRO_FILE_OPEN          SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MAKE_COMPONENT_ENTERED   SET_START_VALUE
 DELETE_SYMBOL            MAKE_COMPONENT_SUSPENDED SHOW_VALUE
 ENTER_SYMBOL             MAP                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       POST                     TABULATE
 EXIT                     READ_WORKSPACES
POLY: s-a-v 1
   ... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(si)
Min value /0/: 0
Max value /1/: .1
Increment /.0025/: .0025
POLY: 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: l-a-v
   ... the command in full is LIST_AXIS_VARIABLE
  Axis No 1: W(SI)                 Min: 0         Max: 0.1       Inc: 2.5E-3
  Axis No 2: T                     Min: 500       Max: 1300      Inc: 10
POLY:@?<Hit_return_to_continue>
POLY: save tcex05 y
   ... the command in full is SAVE_WORKSPACES
POLY: 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-03  6.461E+02
  ** AL2CU_C16
     DIAMOND_A4
     FCC_A1
 Calculated..                     16 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   3.656E-04  5.000E+02
```

```
 ** AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated.                      31 equilibria

Phase region boundary   3 at:   1.067E-02  7.948E+02
 ** LIQUID
 ** AL2CU_C16
    DIAMOND_A4
    FCC_A1

Phase region boundary   4 at:   5.846E-02  7.948E+02
    LIQUID
    AL2CU_C16
 ** DIAMOND_A4
Calculated.                       2 equilibria

Phase region boundary   5 at:   6.069E-02  8.026E+02
    LIQUID
 ** AL2CU_C16
 ** DIAMOND_A4

Phase region boundary   6 at:   6.069E-02  8.026E+02
    LIQUID
 ** DIAMOND_A4
Calculated..                     18 equilibria
Terminating at axis limit.

Phase region boundary   7 at:   6.069E-02  8.026E+02
    LIQUID
 ** AL2CU_C16
Calculated.                       3 equilibria

Phase region boundary   8 at:   5.704E-02  7.964E+02
    LIQUID
 ** AL2CU_C16
 ** FCC_A1

Phase region boundary   9 at:   5.704E-02  7.964E+02
    LIQUID
 ** AL2CU_C16
    FCC_A1
Calculated.                      17 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   5.704E-02  7.964E+02
    LIQUID
 ** FCC_A1
Calculated                      41 equilibria

Phase region boundary  11 at:   5.704E-02  7.964E+02
    LIQUID
    AL2CU_C16
 ** FCC_A1
Calculated.                       2 equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   6.069E-02  8.026E+02
    LIQUID
 ** AL2CU_C16
    DIAMOND_A4
Calculated.                      22 equilibria

Phase region boundary  13 at:   9.890E-02  8.509E+02
    LIQUID
 ** AL2CU_C16
 ** ALCU_ETA
    DIAMOND_A4

Phase region boundary  14 at:   1.058E-01  8.509E+02
 ** LIQUID
    AL2CU_C16
    DIAMOND_A4

Phase region boundary  15 at:   9.890E-02  8.509E+02
    LIQUID
 ** ALCU_ETA
    DIAMOND_A4
Calculated..                       2 equilibria
Terminating at axis limit.

Phase region boundary  16 at:   1.350E-01  8.509E+02
 ** LIQUID
    ALCU_ETA
    DIAMOND_A4

Phase region boundary  17 at:   1.058E-01  8.509E+02
    AL2CU_C16
 ** ALCU_ETA
    DIAMOND_A4

Phase region boundary  18 at:   1.350E-01  8.509E+02
 ** AL2CU_C16
    ALCU_ETA
    DIAMOND_A4

Phase region boundary  19 at:   1.036E-01  7.948E+02
 ** LIQUID
    AL2CU_C16
    DIAMOND_A4

Phase region boundary  20 at:   1.669E-02  7.948E+02
    LIQUID
 ** DIAMOND_A4
    FCC_A1
Calculated.                       4 equilibria

Phase region boundary  21 at:   1.013E-02  7.966E+02
 ** LIQUID
 ** DIAMOND_A4
    FCC_A1

Phase region boundary  22 at:   1.013E-02  7.966E+02
 ** DIAMOND_A4
    FCC_A1
Calculated..                     31 equilibria
```

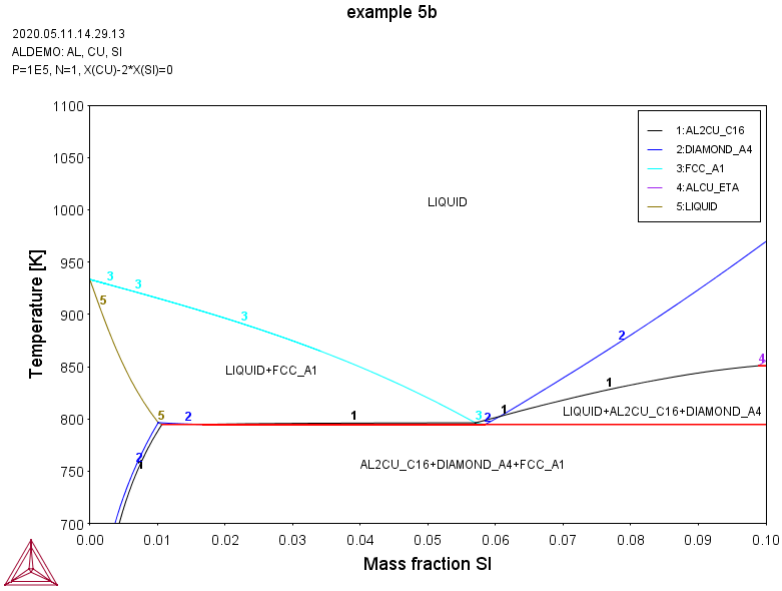
```
Terminating at axis limit.

Phase region boundary  23 at:   1.013E-02  7.966E+02
 ** LIQUID
    FCC_A1
Calculated                     26 equilibria

Phase region boundary  24 at:   1.013E-02  7.966E+02
 ** LIQUID
    DIAMOND_A4
    FCC_A1
Calculated.                     2 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   1.036E-01  7.948E+02
    AL2CU_C16
    DIAMOND_A4
 ** FCC_A1

Phase region boundary  26 at:   2.500E-03  6.461E+02
 ** AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated.                    16 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.417E-02  7.948E+02
 ** LIQUID
    AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated.                    11 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   3.417E-02  7.948E+02
 ** LIQUID
    AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated..                    28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  29 at:   6.583E-02  7.948E+02
 ** LIQUID
    AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated.                    24 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   6.583E-02  7.948E+02
 ** LIQUID
    AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated..                    15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  31 at:   9.750E-02  7.948E+02
 ** LIQUID
    AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated.                    36 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   9.750E-02  7.948E+02
 ** LIQUID
    AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated..                     3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  33 at:   7.899E-03  7.700E+02
 ** DIAMOND_A4
    FCC_A1
Calculated..                    29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  34 at:   7.899E-03  7.700E+02
 ** DIAMOND_A4
    FCC_A1
Calculated.                     4 equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   8.449E-03  7.700E+02
 ** AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated..                    29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  36 at:   8.449E-03  7.700E+02
 ** AL2CU_C16
    DIAMOND_A4
    FCC_A1
Calculated.                     4 equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.500E-03  9.291E+02
    LIQUID
 ** FCC_A1
Calculated                     4 equilibria

Phase region boundary  38 at:   2.500E-03  9.291E+02
    LIQUID
 ** FCC_A1
Calculated.                    23 equilibria
Terminating at known equilibrium
```

```
 Phase region boundary  39 at:   3.417E-02  8.648E+02
     LIQUID
  ** FCC_A1
 Calculated                     26 equilibria

 Phase region boundary  40 at:   3.417E-02  8.648E+02
     LIQUID
  ** FCC_A1
 Calculated.                     11 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   6.583E-02  8.227E+02
     LIQUID
  ** DIAMOND_A4
 Calculated.                      4 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   6.583E-02  8.227E+02
     LIQUID
  ** DIAMOND_A4
 Calculated..                     20 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  43 at:   9.750E-02  9.579E+02
     LIQUID
  ** DIAMOND_A4
 Calculated.                     20 equilibria
 Terminating at known equilibrium

 Phase region boundary  44 at:   9.750E-02  9.579E+02
     LIQUID
  ** DIAMOND_A4
 Calculated..                      4 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex05\tcex05.POLY3
 CPU time for mapping                     12 seconds
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: b
POST:
POST:
POST: set-title example 5a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:@?<Hit_return_to_continue>
POST: s-s y n 700 1100
   ... the command in full is SET_SCALING_STATUS
POST: @@ Note that the three-phase region LIQ-Si-Al2Cu is an area and not
POST: @@ a single line as in a binary system.  This is called a pseudo-binary section
POST: add .05 1000
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Stable phases are: LIQUID
Text size: /.36/:
POST: add .02 840
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
Calculated         17676 grid points in             0 s
 Stable phases are: LIQUID+FCC_A1
Text size: /.36/:
POST: add .04 750
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
```

```
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
Calculated         17676 grid points in             0 s
 Stable phases are: AL2CU_C16+DIAMOND_A4+FCC_A1
Text size: /.36/:
POST: add .07 800
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Testing POLY result by global minimization procedure
Calculated         17676 grid points in             0 s
 Stable phases are: LIQUID+AL2CU_C16+DIAMOND_A4
Text size: /.36/:
POST:
POST: set-title example 5b
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:@?<Hit_return_to_continue>
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex06

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex06\tcex06.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculation of an isopleth in low alloyed
SYS: @@ Fe-Mn-Si-Cr-Ni-C steel.
SYS:
SYS: @@ This example calculates a multicomponent phase diagram using
SYS: @@ the Define_Material command in POLY and the TCFE steel
SYS: @@ database. NA TCFE database license is required to run the
SYS: @@ example.
SYS:
SYS: set-log ex06,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:

POLY: @@ The material contains  1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C
POLY: @@ (by weight). These conditions are set by the command and in
POLY: @@ addition the temperature. Hidden commands set the pressure to 1 bar
POLY: @@ and that iron is "the rest".
POLY: @@ After calculating the first equilibrium we calculate a phase diagram
POLY: @@ with one axis variable as temperature and the other as the
POLY: @@ carbon content
POLY:
POLY: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: tcfe9
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
Major element or alloy: ?
 FILE SYSTEM ERROR IN FILHLP
 ERROR                   1717  READING HELP FILE
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: y
1st alloying element: c
Mass (weight) percent /1/: 1
2nd alloying element: si .3
Next alloying element: mn .4
Next alloying element: ni 3.5
Next alloying element: cr 1.5
Next alloying element:
Temperature (C) /1000/: 1000
 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
 REINITIATING GES .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 NI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 CR  DEFINED


 This database has following phases for the defined system

 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 FE4N_LP1                FECN_CHI                SIGMA
 HIGH_SIGMA              CHI_A12                 LAVES_PHASE_C14
 M3SI                    MN9SI2                  MN11SI19
 MN6SI                   G_PHASE                 CR3SI
 FE2SI                   FESI2_H                 FESI2_L
 MSI                     M5SI3                   NBNI3
 NI3TI                   NB5SI3_D8L              MSI2_C40
 M11SI8                  M6SI5                   AL4C3
 FE8SI2C                 SIC                     MN5SIC
 CRZN17                  CUZN_EPSILON            BETA1
 GAMMA                   AL5FE4                  MP_B31
 M2P_C22                 FLUORITE_C1:I           ZRO2_TETR:I
 M2O3C:I                 M2O3H:I                 CENI2
 CENI5
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                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE                M23C6                    M7C3
 M5C2                     M3C2                     KSI_CARBIDE
 FE4N_LP1                 FECN_CHI                 SIGMA
 HIGH_SIGMA               CHI_A12                  LAVES_PHASE_C14
 M3SI                     MN9SI2                   MN11SI19
 MN6SI                    G_PHASE                  CR3SI
 FE2SI                    FESI2_H                  FESI2_L
 MSI                      M5SI3                    NBNI3
 NI3TI                    NB5SI3_D8L               MSI2_C40
 M11SI8                   M6SI5                    AL4C3
 FE8SI2C                  SIC                      MN5SIC
 CRZN17                   CUZN_EPSILON             BETA1
 GAMMA                    AL5FE4                   MP_B31
 M2P_C22                  FLUORITE_C1:I            ZRO2_TETR:I
 M2O3C:I                  M2O3H:I                  CENI2
 CENI5

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

OK? /Y/: Y
14:30:42,503 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set HCP_A3#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C as it has net charge
Suspending M2O3H as it has net charge
Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE9
      database (TCFE v9.0, Jan, 2017).'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'Unassessed parameter; Linear combination of unary data'
  'A. Fernandez Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362
      (1988); C-CO-NI AND C-CO-FE-NI'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
  'I. Ansara, Unpublished work (1991); Cr-Si'
  'M. Seiersten, Unpublished work (1989); Al-Fe'
  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'C. Qiu, ISIJ International, 32 (1992) 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  '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.-J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  '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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53,
      105-125; Molar volumes'
  'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C
      and Al-Si-C'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
  'Thermo-Calc Software, Sweden, 2019: Volume data updated for TCFE9
      database (TCFE v9.1, June, 2019).'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
  'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6
      database (TCFE v6, April, 2008).'
  'NPL, Unpublished work (1989); C-Mn-Si'
  'W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Intermetallics. 15 (2007)
      1401-1408.'
  'H. Wang, Z. Li, Z. Chen, B. Yang, J. Phase Equilib. Diffus. 37 (2016) 1-7'
```

```
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
       CR-FE-MO'
  'B.-J. Lee, Private communication, (1999); Estimated parameter'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE8
      database (TCFE v8, May, 2015).'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
  'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
  'SGTE (2008): SSOL4 - SGTE Substance Database V4.1, provided by Thermo
      -Calc Software'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
      solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
      same phase as cubic Y2O3 (M2O3C).'
  'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
      and Fe-Mn-Nb'
  'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'L. Zhang, Y. Du, H. Xu, S. Liu, Y. Liu, F. Zheng, et al., Int. J. Mater.
      Res. 100 (2009) 160-175; Fe-Mn-Ni'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
  'S. Liu, Unpublished work (2010); Mn-Ni'
  'C.P. Guo,Intermetallics,13(5),525-534,(2005); Mn-Ni'
  'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
      -21; Mn-Y-O'
  'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
      -64; Mn-Zr-O, Mn-Y-Zr-O'
  'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
  'A. Bolcavage and U.R. Kattner, J. Phase Equilib., 2, (1996); Nb-Ni'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Estimated parameter;
       Ni-Zr-O'
  'P. Bellen, K.C. Hari Kumar and P. Wollants, Z. Metallkd., 87 (1994) 972
      -978; Ni-Ti'
  'J. Miettinen, CALPHAD, 27 (2003) 263-274; Cu-Ni-Zn'
  'H.Liang, Y.A.Chang, J. Phase Equilib. 19 (1998) 25-37'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; C-Cr-Si'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid
      C-Fe-Si description'
  'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
  'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
  'A. Markstrom, Thermo-Calc Software AB, Sweden, 2013; Extrapolations,
      assumptions and adjustment'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Fe-Cr-Ni'
  'J. Miettinen, CALPHAD, 23 (2)(1999) 249-262; Cr-Fe-Si'
  'B.-J. Lee, Private communication, (2000); Estimated parameter'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Fe-Nb-Si'
  'A. Kusoffsky et al., Work within CCT-Applied Stainless steels, 2004; Fe
      -Cr-Si, Fe-Ni-Si, Fe-Cr-Cu, Fe-Cu-Mo, Cr-Mo-N-Ni, Fe-Cr-N-Ni, Fe-Al-Cr
      -Ni'
  'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
      Fe-P-Si'
  'B. Hu, Unpublished (2010); Mn-Ni-Si,Al-Cu-Fe-Ni'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         34730 grid points in             3 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       2 s, total time     5  s
POLY:
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -6.46436E+04,  Enthalpy  3.76393E+04,  Volume  7.13756E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        4.4754E-02  1.0000E-02 8.4968E-02 -2.6099E+04 SER
 CR                       1.5507E-02  1.5000E-02 1.3060E-04 -9.4671E+04 SER
 FE                       8.9803E-01  9.3300E-01 2.4748E-03 -6.3530E+04 SER
 MN                       3.9138E-03  4.0000E-03 3.3096E-06 -1.3358E+05 SER
 NI                       3.2056E-02  3.5000E-02 6.2291E-05 -1.0251E+05 SER
 SI                       5.7417E-03  3.0000E-03 6.4062E-09 -1.9971E+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:Hit RETURN to continue
POLY: @@ Note that values now must be set in fractions and Kelvin.
POLY: 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: s-a-v 2 t
   ... the command in full is SET_AXIS_VARIABLE
Min value /0/: 700
Max value /1/: 1300
Increment /15/:
POLY: save tcex06 y
```

```
   ... the command in full is SAVE_WORKSPACES
POLY: 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:   1.356E-03  7.100E+02
     BCC_A2
     FCC_A1#1
  ** M3C2
     M7C3
 Calculated..                       2 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   1.359E-03  7.000E+02
     BCC_A2
     FCC_A1#1
  ** M3C2
     M7C3
 Calculated.                       3 equilibria

 Phase region boundary   3 at:   1.357E-03  7.212E+02
     BCC_A2
  ** FCC_A1#1
  ** M3C2
     M7C3

 Phase region boundary   4 at:   1.357E-03  7.212E+02
     BCC_A2
  ** M3C2
     M7C3
 Calculated.                      21 equilibria

 Phase region boundary   5 at:   2.406E-03  7.857E+02
     BCC_A2
  ** GRAPHITE
  ** M3C2
     M7C3

 Phase region boundary   6 at:   2.406E-03  7.857E+02
     BCC_A2
     GRAPHITE
  ** M3C2
     M7C3
 Calculated..                      78 equilibria
 Terminating at axis limit.

 Phase region boundary   7 at:   2.406E-03  7.857E+02
     BCC_A2
  ** GRAPHITE
     M7C3
 Calculated.                       7 equilibria

 Phase region boundary   8 at:   2.653E-03  8.656E+02
     BCC_A2
  ** FCC_A1#1
  ** GRAPHITE
     M7C3

 Phase region boundary   9 at:   2.653E-03  8.656E+02
     BCC_A2
     FCC_A1#1
  ** GRAPHITE
     M7C3
 Calculated.                       2 equilibria

 Phase region boundary  10 at:   2.667E-03  8.697E+02
     BCC_A2
  ** CEMENTITE
     FCC_A1#1
```

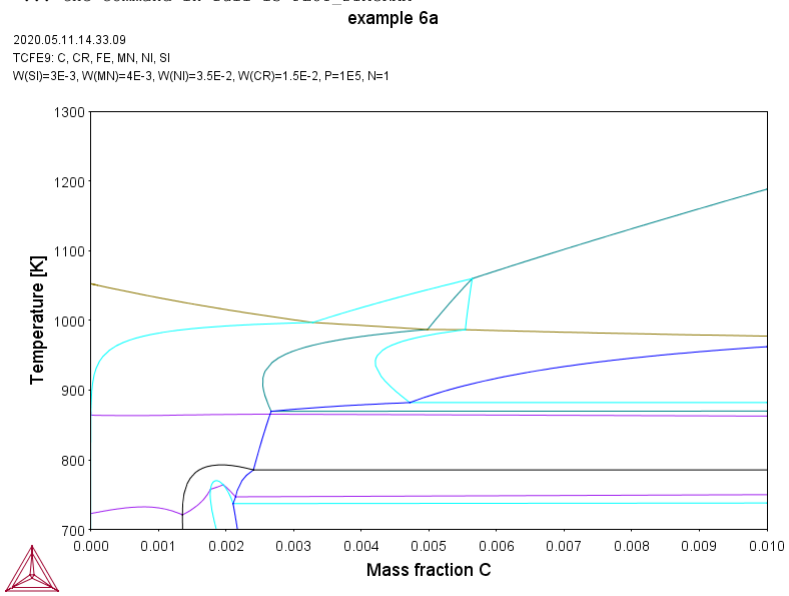
```
 ** GRAPHITE
    M7C3

Phase region boundary  11 at:   2.667E-03  8.697E+02
    BCC_A2
    CEMENTITE
    FCC_A1#1
 ** GRAPHITE
    M7C3
Calculated.                      22 equilibria

Phase region boundary  12 at:   4.718E-03  8.822E+02
    BCC_A2
    CEMENTITE
    FCC_A1#1
 ** GRAPHITE
 ** M7C3

Phase region boundary  13 at:   4.718E-03  8.822E+02
    BCC_A2
    CEMENTITE
    FCC_A1#1
 ** GRAPHITE
Calculated..                      55 equilibria
Terminating at axis limit.

Phase region boundary  14 at:   4.718E-03  8.822E+02
    BCC_A2
    CEMENTITE
    FCC_A1#1
 ** M7C3
Calculated.                      25 equilibria

Phase region boundary  15 at:   5.539E-03  9.866E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1#1
 ** M7C3

Phase region boundary  16 at:   5.539E-03  9.866E+02
    CEMENTITE
    FCC_A1#1
 ** M7C3
Calculated.                       6 equilibria

Phase region boundary  17 at:   5.641E-03  1.060E+03
 ** CEMENTITE
    FCC_A1#1
 ** M7C3

Phase region boundary  18 at:   5.641E-03  1.060E+03
    FCC_A1#1
 ** M7C3
Calculated.                      25 equilibria

Phase region boundary  19 at:   3.284E-03  9.970E+02
 ** BCC_A2
    FCC_A1#1
 ** M7C3

Phase region boundary  20 at:   3.284E-03  9.970E+02
    BCC_A2
    FCC_A1#1
 ** M7C3
Calculated.                      41 equilibria

Phase region boundary  21 at:   2.227E-06  8.642E+02
    BCC_A2
 ** FCC_A1#1
 ** M7C3

Phase region boundary  22 at:   2.227E-06  8.642E+02
    BCC_A2
 ** M7C3
Calculated.                      11 equilibria

Phase region boundary  23 at:   1.481E-08  7.231E+02
    BCC_A2
 ** FCC_A1#2
 ** M7C3

Phase region boundary  24 at:   1.481E-08  7.231E+02
    BCC_A2
    FCC_A1#1
 ** M7C3
Calculated..                       3 equilibria
Terminating at axis limit.

Phase region boundary  25 at:   1.481E-08  7.231E+02
    BCC_A2
 ** FCC_A1#1
Calculated                      13 equilibria

Phase region boundary  26 at:   1.481E-08  7.231E+02
    BCC_A2
 ** FCC_A1#1
    M7C3
Calculated.                      15 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   2.227E-06  8.642E+02
    BCC_A2
 ** FCC_A1#1
Calculated                      19 equilibria

Phase region boundary  28 at:   2.227E-06  8.642E+02
    BCC_A2
 ** FCC_A1#1
    M7C3
Calculated.                      28 equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   3.284E-03  9.970E+02
 ** BCC_A2
    FCC_A1#1
Calculated                      46 equilibria
```

```
Phase region boundary  30 at:   3.284E-03  9.970E+02
 ** BCC_A2
    FCC_A1#1
    M7C3
Calculated.                      18 equilibria

Phase region boundary  31 at:   4.981E-03  9.870E+02
 ** BCC_A2
 ** CEMENTITE
    FCC_A1#1
    M7C3

Phase region boundary  32 at:   4.981E-03  9.870E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1#1
    M7C3
Calculated.                       7 equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   4.981E-03  9.870E+02
 ** CEMENTITE
    FCC_A1#1
    M7C3
Calculated.                      11 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   4.981E-03  9.870E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1#1
    M7C3
Calculated.                      35 equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   5.641E-03  1.060E+03
 ** CEMENTITE
    FCC_A1#1
Calculated..                      46 equilibria
Terminating at axis limit.

Phase region boundary  36 at:   5.539E-03  9.866E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1#1
Calculated..                      47 equilibria
Terminating at axis limit.

Phase region boundary  37 at:   4.718E-03  8.822E+02
    BCC_A2
    CEMENTITE
    FCC_A1#1
    GRAPHITE
 ** M7C3
Calculated..                      55 equilibria
Terminating at axis limit.

Phase region boundary  38 at:   2.667E-03  8.697E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1#1
    GRAPHITE
    M7C3
Calculated..                      76 equilibria
Terminating at axis limit.

Phase region boundary  39 at:   2.653E-03  8.656E+02
    BCC_A2
 ** FCC_A1#1
    GRAPHITE
    M7C3
Calculated..                      76 equilibria
Terminating at axis limit.

Phase region boundary  40 at:   2.406E-03  7.857E+02
    BCC_A2
 ** GRAPHITE
    M3C2
    M7C3
Calculated.                       5 equilibria

Phase region boundary  41 at:   2.142E-03  7.470E+02
    BCC_A2
 ** FCC_A1#1
 ** GRAPHITE
    M3C2
    M7C3

Phase region boundary  42 at:   2.142E-03  7.470E+02
    BCC_A2
    FCC_A1#1
 ** GRAPHITE
    M3C2
    M7C3
Calculated.                       2 equilibria

Phase region boundary  43 at:   2.105E-03  7.373E+02
    BCC_A2
    FCC_A1#1
 ** GRAPHITE
    M3C2
 ** M7C3

Phase region boundary  44 at:   2.105E-03  7.373E+02
    BCC_A2
    FCC_A1#1
 ** GRAPHITE
    M3C2
Calculated..                       4 equilibria
Terminating at axis limit.

Phase region boundary  45 at:   2.105E-03  7.373E+02
    BCC_A2
    FCC_A1#1
    M3C2
```

```
 ** M7C3
Calculated.                      7 equilibria

Phase region boundary  46 at:   1.956E-03  7.645E+02
    BCC_A2
 ** FCC_A1#1
    M3C2
 ** M7C3

Phase region boundary  47 at:   1.956E-03  7.645E+02
    BCC_A2
    M3C2
 ** M7C3
Calculated.                     17 equilibria

Phase region boundary  48 at:   1.772E-03  7.579E+02
    BCC_A2
 ** FCC_A1#2
    M3C2
 ** M7C3

Phase region boundary  49 at:   1.772E-03  7.579E+02
    BCC_A2
    FCC_A1#1
    M3C2
 ** M7C3
Calculated..                      6 equilibria
Terminating at axis limit.

Phase region boundary  50 at:   1.772E-03  7.579E+02
    BCC_A2
 ** FCC_A1#1
    M3C2
Calculated.                      8 equilibria
Terminating at known equilibrium

Phase region boundary  51 at:   1.772E-03  7.579E+02
    BCC_A2
 ** FCC_A1#1
    M3C2
    M7C3
Calculated.                      7 equilibria
Terminating at known equilibrium

Phase region boundary  52 at:   1.956E-03  7.645E+02
    BCC_A2
 ** FCC_A1#1
    M3C2
    M7C3
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary  53 at:   2.105E-03  7.373E+02
    BCC_A2
    FCC_A1#1
    GRAPHITE
    M3C2
 ** M7C3
Calculated..                     81 equilibria
Terminating at axis limit.

Phase region boundary  54 at:   2.142E-03  7.470E+02
    BCC_A2
 ** FCC_A1#1
    GRAPHITE
    M3C2
    M7C3
Calculated..                     81 equilibria
Terminating at axis limit.

Phase region boundary  55 at:   1.356E-03  7.100E+02
    BCC_A2
    FCC_A1#1
 ** M3C2
    M7C3
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  56 at:   1.000E-04  7.249E+02
    BCC_A2
 ** FCC_A1#1
    M7C3
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  57 at:   1.000E-04  7.249E+02
    BCC_A2
 ** FCC_A1#1
    M7C3
Calculated.                     14 equilibria
Terminating at known equilibrium

Phase region boundary  58 at:   3.367E-03  7.374E+02
    BCC_A2
    FCC_A1#1
    GRAPHITE
    M3C2
 ** M7C3
Calculated.                     14 equilibria
Terminating at known equilibrium

Phase region boundary  59 at:   3.367E-03  7.374E+02
    BCC_A2
    FCC_A1#1
    GRAPHITE
    M3C2
 ** M7C3
Calculated..                     69 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  60 at:   6.633E-03  7.378E+02
    BCC_A2
    FCC_A1#1
    GRAPHITE
    M3C2
```

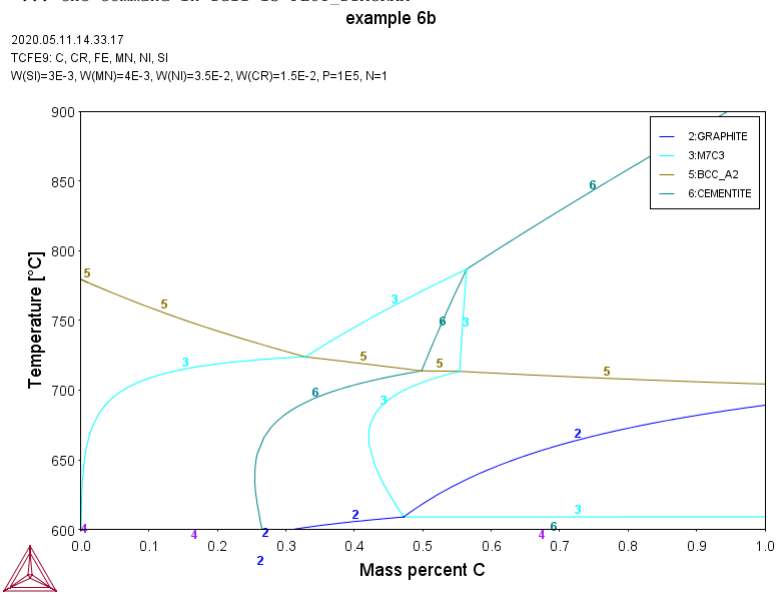
```
 ** M7C3
Calculated.                      47 equilibria
Terminating at known equilibrium

Phase region boundary  61 at:   6.633E-03  7.378E+02
    BCC_A2
    FCC_A1#1
    GRAPHITE
    M3C2
 ** M7C3
Calculated..                      36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  62 at:   2.154E-03  7.100E+02
    BCC_A2
    FCC_A1#1
 ** GRAPHITE
    M3C2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  63 at:   2.154E-03  7.100E+02
    BCC_A2
    FCC_A1#1
 ** GRAPHITE
    M3C2
Calculated.                       3 equilibria
Terminating at known equilibrium

Phase region boundary  64 at:   9.900E-03  7.382E+02
    BCC_A2
    FCC_A1#1
    GRAPHITE
    M3C2
 ** M7C3
Calculated.                      79 equilibria
Terminating at known equilibrium

Phase region boundary  65 at:   9.900E-03  7.382E+02
    BCC_A2
    FCC_A1#1
    GRAPHITE
    M3C2
 ** M7C3
Calculated..                       3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  66 at:   2.549E-03  9.033E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1#1
    M7C3
Calculated.                       4 equilibria
Terminating at known equilibrium

Phase region boundary  67 at:   2.549E-03  9.033E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1#1
    M7C3
Calculated.                      31 equilibria
Terminating at known equilibrium

Phase region boundary  68 at:   5.403E-03  9.033E+02
    BCC_A2
    CEMENTITE
    FCC_A1#1
 ** GRAPHITE
Calculated.                       8 equilibria
Terminating at known equilibrium

Phase region boundary  69 at:   5.403E-03  9.033E+02
    BCC_A2
    CEMENTITE
    FCC_A1#1
 ** GRAPHITE
Calculated..                      48 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  70 at:   6.827E-03  1.097E+03
 ** CEMENTITE
    FCC_A1#1
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  71 at:   6.827E-03  1.097E+03
 ** CEMENTITE
    FCC_A1#1
Calculated..                      34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  72 at:   6.827E-03  1.097E+03
 ** CEMENTITE
    FCC_A1#1
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  73 at:   6.827E-03  1.097E+03
 ** CEMENTITE
    FCC_A1#1
Calculated..                      34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  74 at:   1.000E-04  1.050E+03
 ** BCC_A2
    FCC_A1#1
Calculated                       5 equilibria

Phase region boundary  75 at:   1.000E-04  1.050E+03
 ** BCC_A2
```

```
     FCC_A1#1
 Calculated.                      33 equilibria
 Terminating at known equilibrium

 Phase region boundary  76 at:   3.367E-03  9.996E+02
     FCC_A1#1
  ** M7C3
 Calculated.                       2 equilibria
 Terminating at known equilibrium

 Phase region boundary  77 at:   3.367E-03  9.996E+02
     FCC_A1#1
  ** M7C3
 Calculated.                      24 equilibria
 Terminating at known equilibrium

 Phase region boundary  78 at:   6.633E-03  1.091E+03
  ** CEMENTITE
     FCC_A1#1
 Calculated.                      11 equilibria
 Terminating at known equilibrium

 Phase region boundary  79 at:   6.633E-03  1.091E+03
  ** CEMENTITE
     FCC_A1#1
 Calculated..                      36 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  80 at:   9.900E-03  1.185E+03
  ** CEMENTITE
     FCC_A1#1
 Calculated.                      44 equilibria
 Terminating at known equilibrium

 Phase region boundary  81 at:   9.900E-03  1.185E+03
  ** CEMENTITE
     FCC_A1#1
 Calculated..                        3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex06\tcex06.POLY3
 CPU time for mapping                     52 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST:
POST: set-title example 6a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

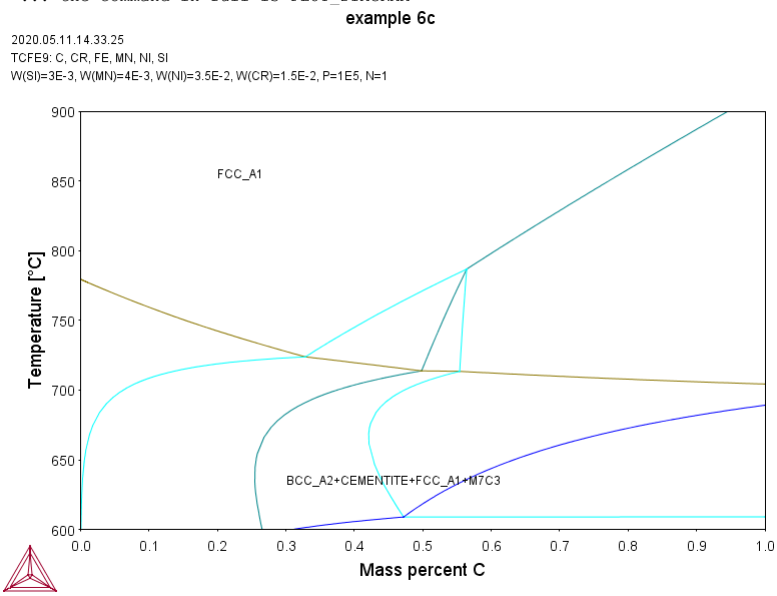



```
POST:
POST:Hit RETURN to continue
POST: @@ Use more practical quantities in the plot and
POST: @@ label the curves
POST: s-d-a x w-p c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST:
POST: s-s y n 600 900
   ... the command in full is SET_SCALING_STATUS
POST:
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
```

```
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Determine the phase region at the iron rich side
POST: add .2 850
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated         34730 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: FCC_A1
Text size: /.36/:
POST: @@ Knowing that only FCC (or austenite) is stable in that region and
POST: @@ which phase is stable along each line, one can determine the phases
POST: @@ in each region. For example at 0.3 % C and 630 degree C one should
POST: @@ have FCC+BCC+M7C3+CEMENTITE.
POST: @@ Check by adding a label
POST:
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         34730 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+CEMENTITE+FCC_A1+M7C3
Text size: /.36/:
POST: s-lab n
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
```

POST:

tcex07

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex07\tcex07.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating single equilibria in low alloyed
SYS: @@ Fe-Mn-Si-Cr-Ni-C steel
SYS:
SYS: @@ There are 2 common ways to perform a single equilibrium
SYS: @@ calculation.
SYS:
SYS: @@ 1) Get data from database, then in POLY use SET_CONDITION
SYS: @@    and COMPUTE_EQUILIBRIUM.
SYS: @@ 2) Go directly to POLY and use DEFINE_MATERIAL.
SYS:
SYS: @@ The COMPUTE_TRANSITION command is also used to determine the
SYS: @@ temperature or composition where one phase forms or
SYS: @@ disappears. It is the same as the CHANGE_STATUS -->
SYS: @@ SET_CONDITION --> COMPUTE_EQUILIBRIUM sequence of commands.
SYS: @@ Note that a TCFE database license is required to run the
SYS: @@ example.
SYS:
SYS: set-log ex07,,
SYS: @@ The alloy composition is 1 wt% Cr, 0.3 wt% Si, 0.3wt% Mn,
SYS: @@ 2.8 wt% Ni and 0.55 wt% C
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: tcfe9
 Current database: Steels/Fe-Alloys  v9.2

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


 This database has following phases for the defined system

 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 FE4N_LP1                FECN_CHI                SIGMA
 HIGH_SIGMA              CHI_A12                 LAVES_PHASE_C14
 M3SI                    MN9SI2                  MN11SI19
 MN6SI                   G_PHASE                 CR3SI
 FE2SI                   FESI2_H                 FESI2_L
 MSI                     M5SI3                   NBNI3
 NI3TI                   NB5SI3_D8L              MSI2_C40
 M11SI8                  M6SI5                   AL4C3
 FE8SI2C                 SIC                     MN5SIC
 CRZN17                  CUZN_EPSILON            BETA1
 GAMMA                   AL5FE4                  MP_B31
 M2P_C22                 FLUORITE_C1:I           ZRO2_TETR:I
 M2O3C:I                 M2O3H:I                 CENI2
 CENI5
Reject phase(s) /NONE/:
Restore phase(s): /NONE/:

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

    The following phases are retained in this system:

 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
```

```
 CEMENTITE                M23C6                    M7C3
 M5C2                     M3C2                     KSI_CARBIDE
 FE4N_LP1                 FECN_CHI                 SIGMA
 HIGH_SIGMA               CHI_A12                  LAVES_PHASE_C14
 M3SI                     MN9SI2                   MN11SI19
 MN6SI                    G_PHASE                  CR3SI
 FE2SI                    FESI2_H                  FESI2_L
 MSI                      M5SI3                    NBNI3
 NI3TI                    NB5SI3_D8L               MSI2_C40
 M11SI8                   M6SI5                    AL4C3
 FE8SI2C                  SIC                      MN5SIC
 CRZN17                   CUZN_EPSILON             BETA1
 GAMMA                    AL5FE4                   MP_B31
 M2P_C22                  FLUORITE_C1:I            ZRO2_TETR:I
 M2O3C:I                  M2O3H:I                  CENI2
 CENI5

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

OK? /Y/: Y
14:34:47,135 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set HCP_A3#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C as it has net charge
Suspending M2O3H as it has net charge
Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE9
      database (TCFE v9.0, Jan, 2017).'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'Unassessed parameter; Linear combination of unary data'
  'A. Fernandez Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362
      (1988); C-CO-NI AND C-CO-FE-NI'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
  'I. Ansara, Unpublished work (1991); Cr-Si'
  'M. Seiersten, Unpublished work (1989); Al-Fe'
  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'C. Qiu, ISIJ International, 32 (1992) 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  '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.-J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  '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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53,
      105-125; Molar volumes'
  'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C
      and Al-Si-C'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
  'Thermo-Calc Software, Sweden, 2019: Volume data updated for TCFE9
      database (TCFE v9.1, June, 2019).'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
  'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6
      database (TCFE v6, April, 2008).'
  'NPL, Unpublished work (1989); C-Mn-Si'
  'W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Intermetallics. 15 (2007)
      1401-1408.'
  'H. Wang, Z. Li, Z. Chen, B. Yang, J. Phase Equilib. Diffus. 37 (2016) 1-7'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
```

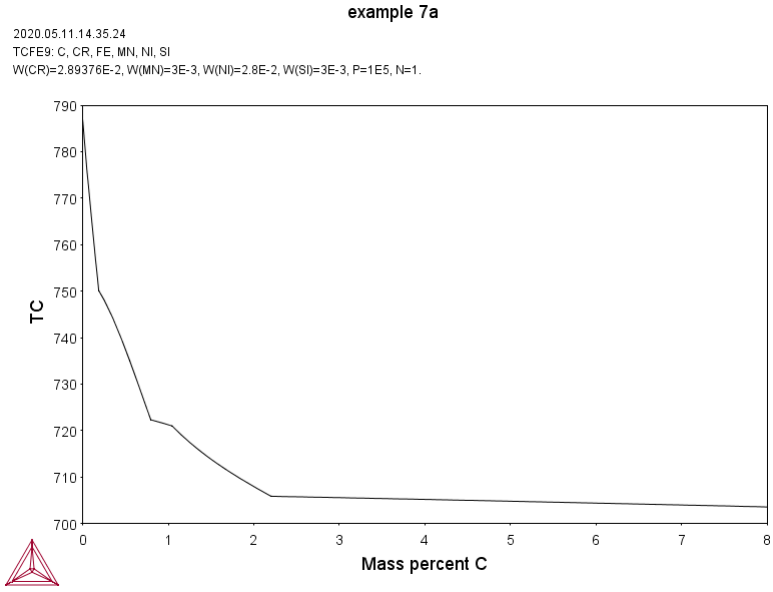
```
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
       CR-FE-MO'
  'B.-J. Lee, Private communication, (1999); Estimated parameter'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE8
      database (TCFE v8, May, 2015).'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
  'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
  'SGTE (2008): SSOL4 - SGTE Substance Database V4.1, provided by Thermo
      -Calc Software'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
      solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
      same phase as cubic Y2O3 (M2O3C).'
  'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
      and Fe-Mn-Nb'
  'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'L. Zhang, Y. Du, H. Xu, S. Liu, Y. Liu, F. Zheng, et al., Int. J. Mater.
      Res. 100 (2009) 160-175; Fe-Mn-Ni'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
  'S. Liu, Unpublished work (2010); Mn-Ni'
  'C.P. Guo,Intermetallics,13(5),525-534,(2005); Mn-Ni'
  'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
      -21; Mn-Y-O'
  'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
      -64; Mn-Zr-O, Mn-Y-Zr-O'
  'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
  'A. Bolcavage and U.R. Kattner, J. Phase Equilib., 2, (1996); Nb-Ni'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Estimated parameter;
       Ni-Zr-O'
  'P. Bellen, K.C. Hari Kumar and P. Wollants, Z. Metallkd., 87 (1994) 972
      -978; Ni-Ti'
  'J. Miettinen, CALPHAD, 27 (2003) 263-274; Cu-Ni-Zn'
  'H.Liang, Y.A.Chang, J. Phase Equilib. 19 (1998) 25-37'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; C-Cr-Si'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid
      C-Fe-Si description'
  'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
  'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
  'A. Markstrom, Thermo-Calc Software AB, Sweden, 2013; Extrapolations,
      assumptions and adjustment'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Fe-Cr-Ni'
  'J. Miettinen, CALPHAD, 23 (2)(1999) 249-262; Cr-Fe-Si'
  'B.-J. Lee, Private communication, (2000); Estimated parameter'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Fe-Nb-Si'
  'A. Kusoffsky et al., Work within CCT-Applied Stainless steels, 2004; Fe
      -Cr-Si, Fe-Ni-Si, Fe-Cr-Cu, Fe-Cu-Mo, Cr-Mo-N-Ni, Fe-Cr-N-Ni, Fe-Al-Cr
      -Ni'
  'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
      Fe-P-Si'
  'B. Hu, Unpublished (2010); Mn-Ni-Si,Al-Cu-Fe-Ni'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         34730 grid points in             2 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       2 s, total time     4  s
POLY:

POLY: @@ The first equilibrium is calculated automatically
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -3.56605E+04,  Enthalpy  1.80235E+04,  Volume  7.20207E-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 3.0096E-04 -5.8867E+04 SER
 FE                       9.2961E-01  9.5050E-01 8.6721E-03 -3.4467E+04 SER
 MN                       2.9826E-03  3.0000E-03 2.8991E-05 -7.5854E+04 SER
 NI                       2.6058E-02  2.8000E-02 3.5045E-04 -5.7761E+04 SER
 SI                       5.8342E-03  3.0000E-03 2.9896E-11 -1.7593E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.5158E-01, Mass 5.3037E+01, Volume fraction 9.6143E-01  Mass fractions:
 FE  9.62930E-01  CR  3.11529E-03  MN  2.11293E-03
 NI  2.87323E-02  SI  3.08953E-03  C   2.02448E-05

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.7166E-02, Mass 7.6060E-01, Volume fraction 1.4311E-02  Mass fractions:
 FE  7.18531E-01  C   6.77699E-02  NI  4.77024E-03
 CR  1.71485E-01  MN  3.74435E-02  SI  4.75410E-13

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.5175E-02, Mass 6.2905E-01, Volume fraction 1.2254E-02  Mass fractions:
 FE  4.74791E-01  C   8.69231E-02  NI  2.93731E-03
 CR  3.98283E-01  MN  3.70657E-02  SI  4.00494E-12

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.6078E-02, Mass 1.9311E-01, Volume fraction 1.2006E-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: ?
```

```
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  GOTO_MODULE              REINITIATE_MODULE
 ADVANCED_OPTIONS         HELP                     SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  INFORMATION              SELECT_EQUILIBRIUM
 BACK                     LIST_AXIS_VARIABLE       SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_CONDITIONS          SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_EQUILIBRIUM         SET_CONDITION
 COMPUTE_TRANSITION       LIST_INITIAL_EQUILIBRIA  SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_STATUS              SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_SYMBOLS             SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
 DEFINE_MATERIAL          MACRO_FILE_OPEN          SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MAKE_COMPONENT_ENTERED   SET_START_VALUE
 DELETE_SYMBOL            MAKE_COMPONENT_SUSPENDED SHOW_VALUE
 ENTER_SYMBOL             MAP                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       POST                     TABULATE
 EXIT                     READ_WORKSPACES
POLY:Hit RETURN to continue
POLY: @@ Increase Cr until all Graphite disappears. Calculate this
POLY: @@ directly using the COMPUTE-TRANSITION command. You
POLY: @@ must release the Cr content
POLY: 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)=.0289376484262
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 Conditions:
 T=873.15, W(C)=5.5E-3, W(CR)=2.89376E-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  5.45447E+01
 Total Gibbs energy -3.61418E+04,  Enthalpy  1.78836E+04,  Volume  7.15511E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        2.4977E-02  5.5000E-03 2.6153E-01 -9.7369E+03 SER
 CR                       3.0356E-02  2.8938E-02 3.0908E-04 -5.8673E+04 SER
 FE                       9.0984E-01  9.3156E-01 8.6672E-03 -3.4471E+04 SER
 MN                       2.9785E-03  3.0000E-03 2.0189E-05 -7.8481E+04 SER
 NI                       2.6022E-02  2.8000E-02 3.6185E-04 -5.7529E+04 SER
 SI                       5.8262E-03  3.0000E-03 3.0998E-11 -1.7567E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.1703E-01, Mass 5.1108E+01, Volume fraction 9.3254E-01  Mass fractions:
 FE  9.62409E-01  CR  3.20855E-03  MN  1.47689E-03
 NI  2.96841E-02  SI  3.20174E-03  C   1.99935E-05

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 8.2972E-02, Mass 3.4369E+00, Volume fraction 6.7455E-02  Mass fractions:
 FE  4.72863E-01  C   8.69900E-02  NI  2.95743E-03
 CR  4.11540E-01  MN  2.56492E-02  SI  4.15471E-12

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 C   1.00000E+00  NI  0.00000E+00  FE  0.00000E+00
 SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Graphite disappears when we have this chromium content 2.94 w/o
POLY: @@ The amount of Cr can be obtained directly with a Show command
POLY: show w(cr)
   ... the command in full is SHOW_VALUE
 W(CR)=2.8937648E-2
POLY: @@ This is automatically set as a new condition by the C-T command
POLY: @@ and the amount of graphite is zero.
POLY: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 M7C3                     ENTERED      0.000000E+00    8.297236E-02
 GRAPHITE                 ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                   ENTERED      0.000000E+00    9.170276E-01
 CEMENTITE                ENTERED     -5.447797E-03    0.000000E+00
 FCC_A1#1                 ENTERED     -2.395219E-02    0.000000E+00
 FCC_A1#2                 ENTERED     -2.395219E-02    0.000000E+00
 M23C6                    ENTERED     -8.104225E-02    0.000000E+00
 M3C2                     ENTERED     -1.333457E-01    0.000000E+00
 HCP_A3#1                 ENTERED     -2.603591E-01    0.000000E+00
 HCP_A3#2                 ENTERED     -2.603591E-01    0.000000E+00
 M5C2                     ENTERED     -2.797331E-01    0.000000E+00
 FECN_CHI                 ENTERED     -3.871871E-01    0.000000E+00
 CUB_A13                  ENTERED     -5.374101E-01    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -6.884393E-01
 LIQUID SIGMA CHI_A12 DIAMOND_FCC_A4 CBCC_A12 LAVES_PHASE_C14 FE4N_LP1 AL5FE4
 KSI_CARBIDE CRZN17 FE8SI2C G_PHASE M3SI GAMMA NI3TI FE2SI NBNI3 CENI2 CENI5
 BETA1 CR3SI M2P_C22 M5SI3 MN5SIC HIGH_SIGMA MN6SI MN9SI2 CUZN_EPSILON MSI
 MP_B31 SIC M6SI5 FESI2_L AL4C3 MN11SI19 MSI2_C40 FESI2_H M11SI8 NB5SI3_D8L
 GAS
POLY: @@ Now determine the maximum temperature with no Austenite (FCC_A1),
POLY: @@ i.e. A1 temperature.
POLY: @@ Use the command COMPUTE-TRANSITION again
POLY: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: fcc_a1
 You must release one of these conditions
 T=873.15, W(C)=5.5E-3, W(CR)=2.89376E-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         34730 grid points in             0 s
```

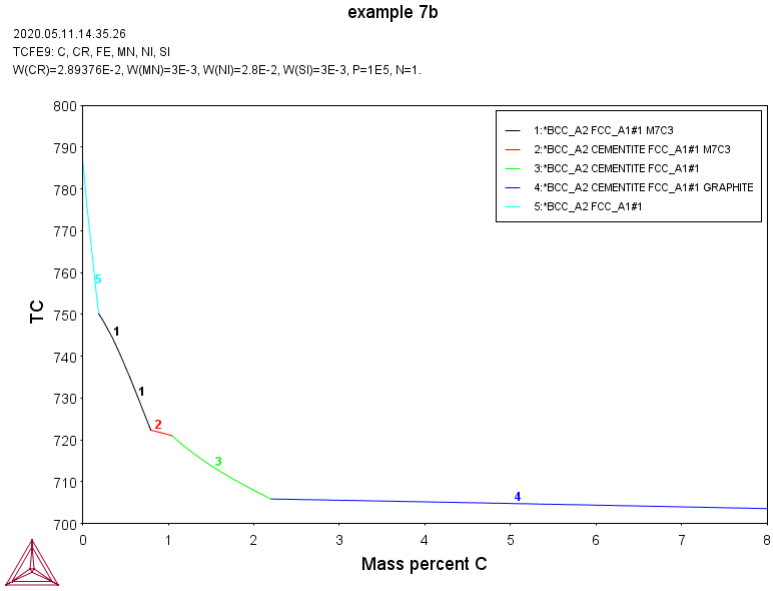
```
To form FCC_A1 the condition is set to T=923.305059564
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=923.305, W(C)=5.5E-3, W(CR)=2.89376E-2, W(MN)=3E-3, W(NI)=2.8E-2,
    W(SI)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY: @@ This command does the same as Change-Status/Set-Cond/Compute-Equil sequence.
POLY: @@ Notice that the temperature is set back as condition with the new value.
POLY: @@ If we want temperatures in Celsius enter a function.
POLY: ent fun tc=t-273;
   ... the command in full is ENTER_SYMBOL
POLY: sh tc
   ... the command in full is SHOW_VALUE
 TC=650.30506
POLY:Hit RETURN to continue
POLY:
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 Conditions:
 T=923.305, W(C)=5.5E-3, W(CR)=2.89376E-2, W(MN)=3E-3, W(NI)=2.8E-2,
    W(SI)=3E-3, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature    923.31 K (   650.16 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45447E+01
 Total Gibbs energy -3.93091E+04,  Enthalpy  2.01926E+04,  Volume  7.17239E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.4977E-02  5.5000E-03 2.0363E-01 -1.2217E+04 SER
 CR                      3.0356E-02  2.8938E-02 3.2335E-04 -6.1697E+04 SER
 FE                      9.0984E-01  9.3156E-01 7.4671E-03 -3.7595E+04 SER
 MN                      2.9785E-03  3.0000E-03 1.6904E-05 -8.4353E+04 SER
 NI                      2.6022E-02  2.8000E-02 2.8547E-04 -6.2653E+04 SER
 SI                      5.8262E-03  3.0000E-03 7.3351E-11 -1.7914E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.1644E-01, Mass 5.1066E+01, Volume fraction 9.3201E-01  Mass fractions:
 FE  9.60789E-01  CR  4.50578E-03  MN  1.76523E-03
 NI  2.96964E-02  SI  3.20435E-03  C   3.90651E-05

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 7.8408E-02, Mass 3.2502E+00, Volume fraction 6.3662E-02  Mass fractions:
 FE  4.86783E-01  C   8.69252E-02  NI  2.97527E-03
 CR  4.02197E-01  MN  2.11195E-02  SI  1.22958E-11

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 5.1532E-03, Mass 2.2825E-01, Volume fraction 4.3267E-03  Mass fractions:
 FE  7.26232E-01  C   6.77936E-02  NI  4.80781E-03
 CR  1.79929E-01  MN  2.12374E-02  SI  4.75577E-13

 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  8.81899E-01  MN  1.00709E-02  SI  3.88059E-03
 NI  9.43559E-02  CR  7.11210E-03  C   2.68170E-03
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: cps
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 NI                      ENTERED   SER
 SI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 M7C3                    ENTERED      0.000000E+00    7.840801E-02
 FCC_A1#2                ENTERED      0.000000E+00    0.000000E+00
 FCC_A1#1                ENTERED      0.000000E+00    0.000000E+00
 CEMENTITE               ENTERED      0.000000E+00    5.153158E-03
 BCC_A2                  ENTERED      0.000000E+00    9.164388E-01
 M23C6                   ENTERED     -6.440111E-02    0.000000E+00
 GRAPHITE                ENTERED     -1.782678E-01    0.000000E+00
 M3C2                    ENTERED     -2.004382E-01    0.000000E+00
 HCP_A3#1                ENTERED     -2.483487E-01    0.000000E+00
 HCP_A3#2                ENTERED     -2.483487E-01    0.000000E+00
 M5C2                    ENTERED     -2.793270E-01    0.000000E+00
 FECN_CHI                ENTERED     -3.895429E-01    0.000000E+00
 CUB_A13                 ENTERED     -4.940212E-01    0.000000E+00
 LIQUID                  ENTERED     -5.797545E-01    0.000000E+00
 SIGMA                   ENTERED     -6.216510E-01    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -6.374932E-01
 CHI_A12 CBCC_A12 LAVES_PHASE_C14 FE4N_LP1 AL5FE4 DIAMOND_FCC_A4 KSI_CARBIDE
 CRZN17 FE8SI2C G_PHASE M3SI GAMMA FE2SI NI3TI CR3SI M2P_C22 CENI5 NBNI3 CENI2
 M5SI3 BETA1 MN5SIC HIGH_SIGMA MN6SI MSI MN9SI2 CUZN_EPSILON MP_B31 SIC M6SI5
 FESI2_L AL4C3 MN11SI19 MSI2_C40 FESI2_H M11SI8 NB5SI3_D8L GAS
 *** STATUS FOR ALL SPECIES
 C    ENTERED    C60  ENTERED    FE+2 ENTERED    MN+3 ENTERED    SI   ENTERED
 C2   ENTERED    CR   ENTERED    FE+3 ENTERED    MN+4 ENTERED    SI+4 ENTERED
 C3   ENTERED    CR+2 ENTERED    FE+4 ENTERED    NI   ENTERED    VA   ENTERED
 C4   ENTERED    CR+3 ENTERED    MN   ENTERED    NI+2 ENTERED
 C5   ENTERED    FE   ENTERED    MN+2 ENTERED    NI+3 ENTERED
POLY: @@ Now determine maximum temperature where no Ferrite (BCC_A2) exists
POLY: @@ Use
POLY: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
You want to find when the current major phase is formed, please give
New major phase: fcc_a1
 You must release one of these conditions
 T=923.305, W(C)=5.5E-3, W(CR)=2.89376E-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         34730 grid points in             0 s
To form BCC_A2 the condition is set to T=1007.99583472
POLY:
```

```
POLY: show tc
   ... the command in full is SHOW_VALUE
 TC=734.99583
POLY:Hit RETURN to continue
POLY: @@ Check how this varies with the carbon content
POLY: ch-st phase fcc_a1
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: ent
Start value, number of mole formula units /0/: 1
POLY: ch-st phase bcc_a2
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: fix
Number of mole formula units /0/: 0
POLY:
POLY: s-c t=none
   ... the command in full is SET_CONDITION
POLY:
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
     7 ITS,  CPU TIME USED   0 SECONDS
POLY: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 Conditions:
 W(C)=5.5E-3, W(CR)=2.89376E-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   1008.00 K (   734.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.45447E+01
 Total Gibbs energy -4.50506E+04,  Enthalpy  2.77286E+04,  Volume  7.08290E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.4977E-02  5.5000E-03 8.8252E-02 -2.0345E+04 SER
 CR                      3.0356E-02  2.8938E-02 5.0800E-04 -6.3570E+04 SER
 FE                      9.0984E-01  9.3156E-01 5.8584E-03 -4.3077E+04 SER
 MN                      2.9785E-03  3.0000E-03 4.9655E-06 -1.0236E+05 SER
 NI                      2.6022E-02  2.8000E-02 8.2581E-05 -7.8796E+04 SER
 SI                      5.8262E-03  3.0000E-03 3.4411E-10 -1.8262E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.6534E-01, Mass 5.3116E+01, Volume fraction 9.7135E-01  Mass fractions:
 FE  9.45237E-01  CR  1.67099E-02  SI  3.08069E-03
 NI  2.87274E-02  C   3.29654E-03  MN  2.94880E-03

 M7C3                        Status ENTERED     Driving force  0.0000E+00
 Moles 3.4662E-02, Mass 1.4287E+00, Volume fraction 2.8650E-02  Mass fractions:
 CR  4.83535E-01  C   8.74192E-02  NI  9.58198E-04
 FE  4.23184E-01  MN  4.90349E-03  SI  6.67300E-11

 BCC_A2                      Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.70897E-01  CR  1.12377E-02  MN  9.29098E-04
 NI  1.30455E-02  SI  3.80828E-03  C   8.20033E-05
POLY: show tc
   ... the command in full is SHOW_VALUE
 TC=734.99583
POLY:
POLY:Hit RETURN to continue
POLY:
POLY: s-a-v 1 w(c) 0 .08 0.001,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex07 y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.550000E-02
...OK

 Phase Region from   0.550000E-02 for:
     BCC_A2
     FCC_A1#1
     M7C3
 Global check of adding phase at  7.95772E-03
 Calculated     5 equilibria

 Phase Region from   0.795772E-02 for:
     BCC_A2
     CEMENTITE
     FCC_A1#1
     M7C3
 Global check of removing phase at  1.04363E-02
 Calculated     5 equilibria

 Phase Region from   0.104363E-01 for:
     BCC_A2
     CEMENTITE
     FCC_A1#1
 Global test at  1.85000E-02 .... OK
 Global check of adding phase at  2.20196E-02
 Calculated    14 equilibria

 Phase Region from   0.220196E-01 for:
     BCC_A2
     CEMENTITE
     FCC_A1#1
     GRAPHITE
 Global test at  2.95000E-02 .... OK
 Global test at  3.95000E-02 .... OK
 Global test at  4.95000E-02 .... OK
 Global test at  5.95000E-02 .... OK
 Global test at  6.95000E-02 .... OK
 Global test at  7.95000E-02 .... OK
 Terminating at   0.800000E-01
 Calculated    62 equilibria

 Phase Region from   0.550000E-02 for:
     BCC_A2
     FCC_A1#1
```

```
     M7C3
 Global check of removing phase at  1.87793E-03
 Calculated     6 equilibria

 Phase Region from   0.187793E-02 for:
     BCC_A2
     FCC_A1#1
 Global test at  9.99743E-16 .... OK
 Terminating at   0.215887E-12
 Calculated     6 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex07\tcex07.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x w-p c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y tc
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 7a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-s y n 700 800
   ... the command in full is SET_SCALING_STATUS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 7b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex08

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex08\tcex08.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculation of a property diagram for a high speed steel
SYS:
SYS: @@ This example shows how to calculate property diagrams
SYS: @@ for a high speed steel i.e. phase fraction plots,
SYS: @@ activity vs temperature, and so forth.
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex08,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: 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
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: tcfe9
 Current database: Steels/Fe-Alloys  v9.2

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


 This database has following phases for the defined system

 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
 SIGMA                   HIGH_SIGMA              MU_PHASE
 P_PHASE                 R_PHASE                 CHI_A12
 LAVES_PHASE_C14         M3SI                    MN9SI2
 MN11SI19                MN6SI                   G_PHASE
 CR3SI                   FE2SI                   FESI2_H
 FESI2_L                 MSI                     M5SI3
 CO3VV                   MOSI2_C11B              MO5SI3_D8M
 NB5SI3_D8L              MSI2_C40                M11SI8
 M6SI5                   AL4C3                   FE8SI2C
 SIC                     MN5SIC                  CRZN17
 CUZN_EPSILON            AL5FE4                  MP_B31
 M2P_C22                 FLUORITE_C1:I           ZRO2_TETR:I
 M2O3C:I                 M2O3H:I
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                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
```

```
 SIGMA                    HIGH_SIGMA               MU_PHASE
 P_PHASE                  R_PHASE                  CHI_A12
 LAVES_PHASE_C14          M3SI                     MN9SI2
 MN11SI19                 MN6SI                    G_PHASE
 CR3SI                    FE2SI                    FESI2_H
 FESI2_L                  MSI                      M5SI3
 CO3VV                    MOSI2_C11B               MO5SI3_D8M
 NB5SI3_D8L               MSI2_C40                 M11SI8
 M6SI5                    AL4C3                    FE8SI2C
 SIC                      MN5SIC                   CRZN17
 CUZN_EPSILON             AL5FE4                   MP_B31
 M2P_C22                  FLUORITE_C1:I            ZRO2_TETR:I
 M2O3C:I                  M2O3H:I

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

OK? /Y/: Y
14:36:46,839 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set HCP_A3#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C as it has net charge
Suspending M2O3H as it has net charge
Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE9
      database (TCFE v9.0, Jan, 2017).'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'J-O. Andersson, CALPHAD, 12 (1988) 1-8; TRITA 0317 (1986); C-MO'
  'Unassessed parameter; Linear combination of unary data'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
  'I. Ansara, Unpublished work (1991); Cr-Si'
  'J. Bratberg and B. Sundman, J. Phase Equilib., 24, No. 6, 2003, 495-503;
      Co-V'
  'J. Bratberg and Karin Frisk, CALPHAD, 26, No. 3, 459-476, 2002; Mo-V-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2015; LAVES_PHASE_C14'
  'B.-J. Lee, Private communication, (1999); Estimated parameter'
  'P. Gustafson, Z. Metallkd., 79 (1988) 397-402; TRITA-MAC 330 (1987); C-MO
      -W'
  'M. Seiersten, Unpublished work (1989); Al-Fe'
  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'C. Qiu, ISIJ International, 32 (1992) 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  '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.-J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  '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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'J.-H. Shim, C.-S. Oh, D.N. Lee, Metall. Mater. Trans. B. 27 (1996) 955
      -966; Ti-Mo-C'
  'Thermo-Calc Software, Sweden, 2019: Volume data updated for TCFE9
      database (TCFE v9.1, June, 2019).'
  'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C
      and Al-Si-C'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
  'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6
      database (TCFE v6, April, 2008).'
  'NPL, Unpublished work (1989); C-Mn-Si'
  'W. Huang, TRITA-MAC 431 (1990); C-V'
  'A. Fernandez Guillermet and W. Huang, TRITA-MAC 440 (1990); Mn-V-C'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53,
      105-125; Molar volumes'
  'B.-J. Lee, TRITA-MAC 475 (1991); C-Cr-Fe-V'
  'A. Fernandez Guillermet, Z. Metallkd. 82 (1991) 478-487; Nb-Zr'
  'S. Jonsson, PhD Thesis; TRITA-MAC 519 (1993); W-C and Ti-W-C'
  'P. Gustafson, Mat. Sci. Tech., 2 (1986) 653-658; TRITA 0212 (1985); C-W'
  'P. Gustafson, Metall. Trans. A, 18A (1987) 175-188; TRITA 0257 (1985); C
      -FE-W'
```

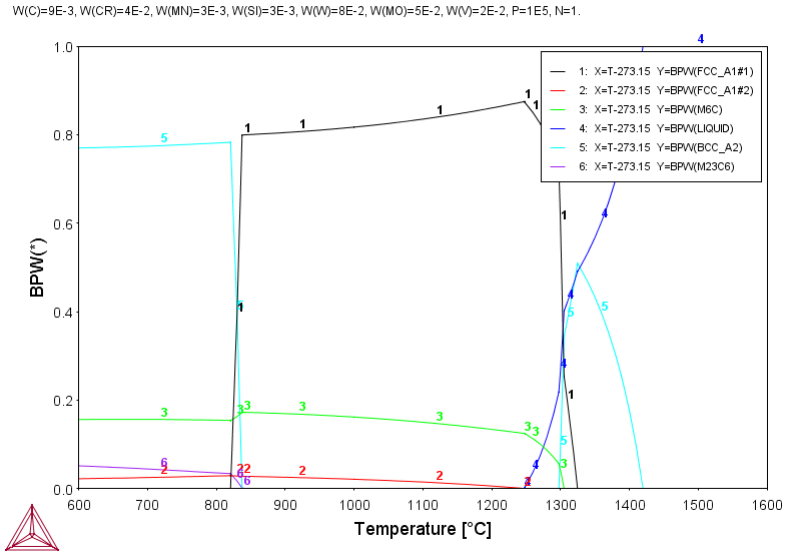
'P. Gustafson, Z. Metallkd., 79 (1988) 421-425; TRITA-MAC 331 (1987); C -FE-MO-W'
'N. Dupin, Private communication; Introduction of V'
'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270 (1986); CR-FE'
'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR -FE-N'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986); CR-FE-MO'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE8 database (TCFE v8, May, 2015).'
'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
'SGTE (2008): SSOL4 - SGTE Substance Database V4.1, provided by Thermo -Calc Software'
'K. Frisk, KTH Report D 60 (1984); CR-MO'
'B. Sundman, Private communication; FCC parameter same as BCC; Cr-Mo'
'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Z_PHASE'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the same phase as cubic Y2O3 (M2O3C).'
'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
'B.-J. Lee, TRITA-MAC 474 (1991); Cr-Fe-V'
'H.K. Danielsen and J. Hald, CALPHAD, 31 (2007) 505-514; Z-PHASE'
'P. Gustafson, CALPHAD, 11 (1987) 277-292; TRITA-MAC 320 (1986); CR-NI-W '
'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb and Fe-Mn-Nb'
'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
'A. Fernandez Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised 1986); TRITA-MAC 200 (1982); FE-MO'
'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe -Si-C'
'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
'W. Huang, TRITA-MAC 432 (Rev 1989,1990); FE-V'
'J-O. Andersson, CALPHAD, 7 (1983) 305-315 (Parameters revised 1986 due to new decription of V) TRITA 0201 (1982); FE-V'
'W. Huang, TRITA-MAC 432 (1990); C-Fe-V'
'A.V. Khvan, K. Chang, B. Hallstedt, CALPHAD, 43, 143-48(2013); Fe-Nb-V'
'W. Huang, TRITA-MAC 439 (1990) also in W. Huang, CALPHAD, 15, 195 -208(1991); Mn-V, Fe-Mn-V'
'P. Gustafson, Z. Metallkd., 79 (1988) 388-396; TRITA-MAC 329 (1987); MO-W, FE-MO-W '
'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114 -21; Mn-Y-O'
'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457 -64; Mn-Zr-O, Mn-Y-Zr-O'
'W. Huang, TRITA-MAC 441 (1990) also in W. Huang, Metall. Trans. A, 22A, 1911-20(1991); Fe-Mn-V-C'
'COST2 database 1997'
'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
'Y. Liu, G. Shao, P. Tsakiropoulos, Intermatallics 8 (2000) 953-962; Mo-Si, Al-Mo-Si'
'M.H. Rand and N. Saunders, COST 507 Report (1998); Si-V'
'C. Vahlas, P-Y. Chevalier and E. Blanquet, CALPHAD, 13 (1989) 273-292; Mo -Si and Si-W'
'S. Huang, J. Vleugels, L. Li, O. Van Der Biest, J. Alloys Compd., 395 (2005) 68-74; V-W-C'
'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C -CR-FE'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-V-W-C'
'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; C-Cr-Si'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and M23C6'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-V-C'
'S. Nagakura, Transactions of the Iron and Steel Institute of Japan, 8 (1968) 265-294; Molar volumes'
'I.K. Kupalova, V.I. Pavlova, High Speed Steels: Physical Properties, Prop. Data Updat. 2 (1988) 67-78; Molar volumes'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid C-Fe-Si description'
'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
'A. Markstrom, Thermo-Calc Software AB, Sweden, 2013; Extrapolations, assumptions and adjustment'
'B. Sundman, Private communication, (2000); Estimated Cr-Ni-Mo'
'B.-J. Lee, Private communication, (2000); Estimated parameter'
'J. Miettinen, CALPHAD, 23 (2)(1999) 249-262; Cr-Fe-Si'
'A. Markstrom, Thermo-calc Software AB, Sweden, 2011; SIGMA phase in Cr-Fe -W'
'J. Miettinen, CALPHAD, 22 (1998) 275-300; Fe-Mo-Si'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Fe-Nb-Si'
'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290; Fe-P-Si'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; C-Cr-Fe-V'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; C-Cr-Fe-W'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Solubilities in M6C'
'P. Gustafson, Inst. Met. Res. (Sweden) (1990); Estimations of C-CR-FE-V, C-CR-FE-MO-V-W, FE-N-W, FE-MN-N, FE-N-SI, CR-N-V, C-CR-N, FE-MO-N, CR -N-W, CR-TI-N'
-OK-

Should any phase have a miscibility gap check? /N/: N

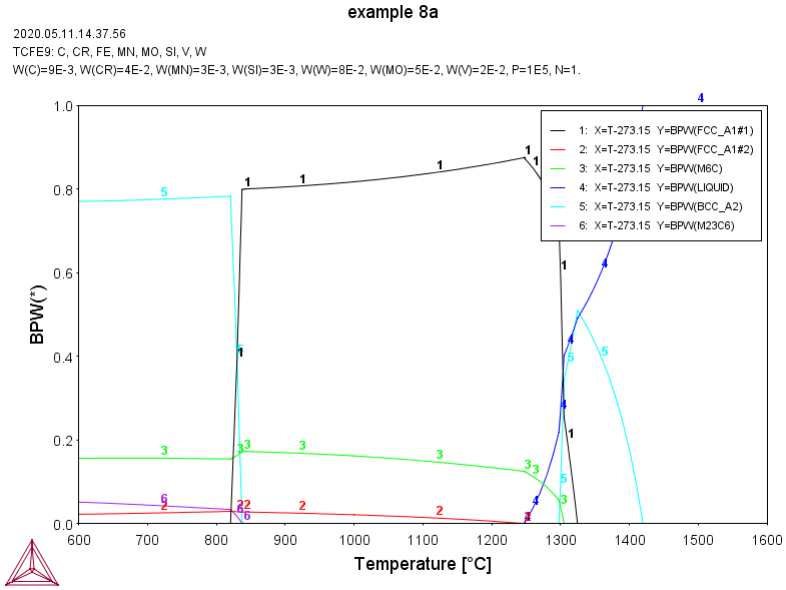
```
 Using global minimization procedure
Calculated         45329 grid points in             3 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       3 s, total time     6  s
 You must now set an independent axis for your diagram
 as one of the following conditions:
 Condition  1 is temperature (Celsius)
 Condition  2 is mass percent of C
 Condition  3 is mass percent of CR
 Condition  4 is mass percent of MN
 Condition  5 is mass percent of SI
 Condition  6 is mass percent of W
 Condition  7 is mass percent of MO
 Condition  8 is mass percent of V
```

```
Give the number of the condition to vary /1/: 1
Minimum value (C) /800/: 600
Maximum value (C) /1800/: 1600

 The second axis can be another of the conditions above and you will then
 calculate a phase diagram.
 Or you may want to plot how some other quantities depend on the selected
 condition and you will then calculate a  "property" diagram.

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

 Phase Region from    1273.15     for:
     FCC_A1#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  1.52101E+03
 Calculated    27 equilibria

 Phase Region from    1521.01     for:
     LIQUID
     FCC_A1#1
     FCC_A1#2
     M6C
 Global check of removing phase at  1.52118E+03
 Calculated     3 equilibria

 Phase Region from    1521.18     for:
     LIQUID
     FCC_A1#1
     M6C
 Global check of adding phase at  1.57077E+03
 Calculated     8 equilibria

 Phase Region from    1570.77     for:
     LIQUID
     BCC_A2
     FCC_A1#1
     M6C
 Global check of removing phase at  1.57833E+03
 Calculated     4 equilibria

 Phase Region from    1578.33     for:
     LIQUID
     BCC_A2
     FCC_A1#1
 Global check of removing phase at  1.59788E+03
 Calculated     5 equilibria

 Phase Region from    1597.88     for:
     LIQUID
     BCC_A2
 Global test at  1.67315E+03 .... OK
 Global check of removing phase at  1.69303E+03
 Calculated    12 equilibria

 Phase Region from    1693.03     for:
     LIQUID
 Global test at  1.76315E+03 .... OK
 Global test at  1.86315E+03 .... OK
 Terminating at    1873.15
 Calculated    22 equilibria

 Phase Region from    1273.15     for:
     FCC_A1#1
     FCC_A1#2
     M6C
 Global test at  1.19315E+03 .... OK
 Global check of adding phase at  1.11546E+03
 Calculated    18 equilibria

 Phase Region from    1115.46     for:
     FCC_A1#1
     FCC_A1#2
     M23C6
     M6C
 Global check of adding phase at  1.11050E+03
 Calculated     4 equilibria

 Phase Region from    1110.50     for:
     BCC_A2
     FCC_A1#1
     FCC_A1#2
     M23C6
     M6C
 Global check of removing phase at  1.09373E+03
 Calculated     4 equilibria

 Phase Region from    1093.73     for:
     BCC_A2
     FCC_A1#2
     M23C6
     M6C
 Global test at  1.02315E+03 .... OK
 Global test at  9.23150E+02 .... OK
 Terminating at    873.150
 Calculated    26 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex08\tcex08.POLY3
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

   ... the command in full is REINITIATE_PLOT_SETTINGS
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes
```

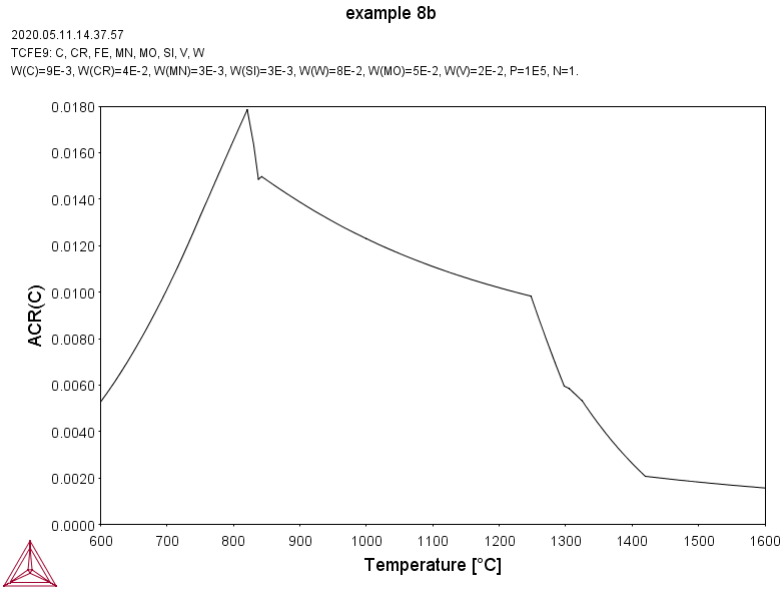
```
   ... the command in full is SET_AUTOMATIC_DIAGRAM_A

 Setting automatic diagram axes

   ... the command in full is PLOT_DIAGRAM
```



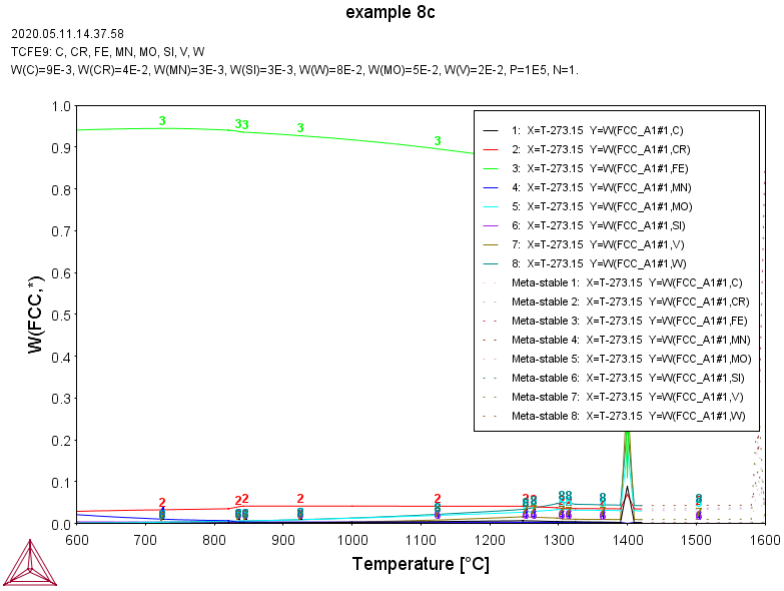

```
POST:
POST:Hit RETURN to continue
POST: set-title example 8a
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



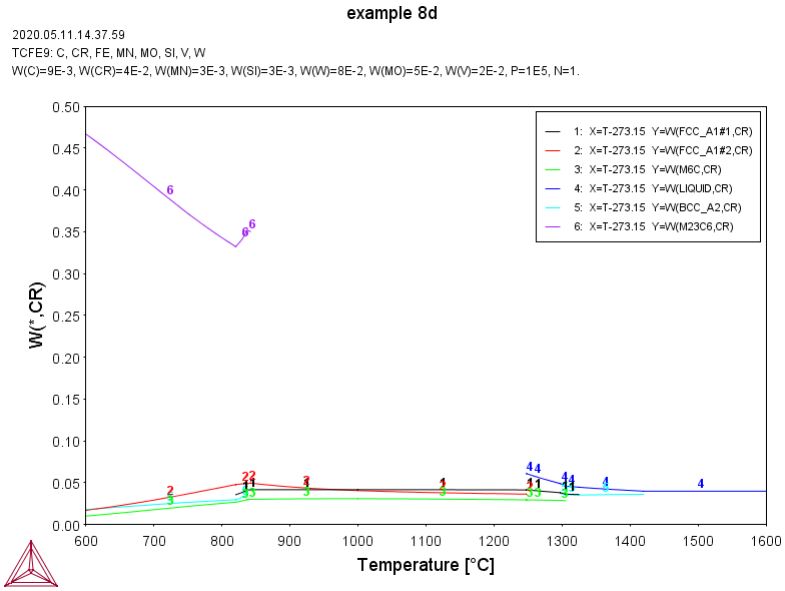

```
POST:
POST:Hit RETURN to continue
POST: s-d-a y acr(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set_lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: n
POST: set-title example 8b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the composition of the austenite (called fcc) varies
POST: @@ Note this is plotted also where the austenite is not stable.
POST: s-d-a y w(fcc,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set_lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 8c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the fraction of Cr in all phases
POST: s-d-a y w(*,cr)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 8d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



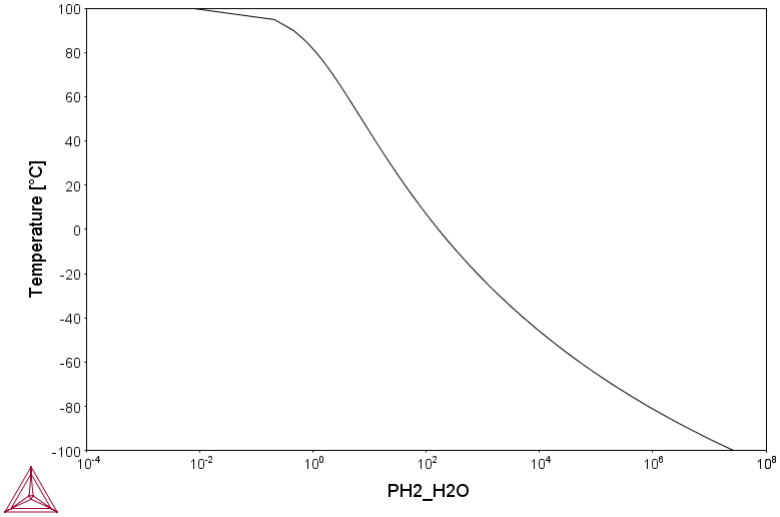

```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex09

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex09\tcex09.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a dew point with the POLY3 module
SYS:
SYS: go data
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw subdemo
 Current database: Substance Demo Database v1.0

 VA                      /-  DEFINED
TDB_SUBDEMO: def-sp h2 h2o1
 H2                      H2O1  DEFINED
TDB_SUBDEMO: get
14:39:24,070 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'H2<G> JANAF THERMOCHEMICAL TABLES SGTE ** H2<G> H2<G> HYDROGEN<G>
      STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61'
  'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
  'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
 -OK-
TDB_SUBDEMO: go p-3

 POLY version  3.32
POLY: s-c n=1 p=1e5 t=233
POLY: ch-st ph h2o_l=f 0
POLY: c-e
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           210 grid points in             0 s
    22 ITS,  CPU TIME USED   0 SECONDS
POLY: l-e,,,
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 N=1, P=1E5, T=233
 FIXED PHASES
 H2O1_L=0
 DEGREES OF FREEDOM 0

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

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 H                       9.9991E-01  9.9851E-01 3.6499E-04 -1.5335E+04 SER
 O                       9.3929E-05  1.4889E-03 1.0377E-61 -2.7203E+05 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0093E+00, Volume fraction 1.0000E+00  Mass fractions:
 H  9.98511E-01  O  1.48890E-03
 Constitution:
 H2    9.99812E-01  H2O1  1.87875E-04

 H2O1_L                      Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O  8.88103E-01  H  1.11897E-01
POLY: ent fun ph2_h2o=acr(h2,gas)/acr(h2o,gas);
POLY: s-a-v 1 t 173.15 373.15 ,
POLY: save dew y
POLY: step normal
 No initial equilibrium, using default
 Step will start from axis value    233.000
...OK

 Phase Region from    233.000     for:
     GAS
     H2O1_L
 Global test at  2.73000E+02 .... OK
 Global test at  3.23000E+02 .... OK
 Global test at  3.73000E+02 .... OK
 Terminating at    373.150
 Calculated    32 equilibria

 Phase Region from    233.000     for:
     GAS
     H2O1_L
 Global test at  1.93000E+02 .... OK
 Terminating at    173.150
 Calculated    15 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex09\dew.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
```

```
 Setting automatic diagram axes

POST: s-d-a x ph2_h2o
POST: s-a-ty x log
POST: s-d-a y t-c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

2020.05.11.14.39.28
SUBDEMO: H, O
N=1., P=1E5




```
POST:
POST:
POST: set-inter
POST:
```

tcex10

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex10\tcex10.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Preventing Cr2O3 clogging in a continuous casting process
SYS:
SYS: @@ This example calculates an equilibrium with suspended or
SYS: @@ dormant phases and shows how to avoid Cr2O3 clogging in
SYS: @@ a continuous casting process.
SYS: @@ Note that a license for the SLAG database is required to
SYS: @@ run the example.
SYS:
SYS: @@ The background to this example is that a manufacturer
SYS: @@ wanted to increase the Cr content of a material from 18
SYS: @@ to 25 weight percent. He then had trouble in the continous
SYS: @@ casting of this material because solid Cr2O3 was formed.
SYS: @@ By calculating the equilibria in the steel/slag system a
SYS: @@ simple correction could be found: modify the Mn or Si
SYS: @@ content, thus decrease the oxygen potential.
SYS:
SYS: @@ In Thermo-Calc, you can FIX a phase with zero amount to
SYS: @@ simulate how to avoid forming this phase. You can then
SYS: @@ release one of the conditions, usually one of the
SYS: @@ compositions, and this composition is determined by the
SYS: @@ equilibrium calculation.
SYS:
SYS: set-log ex10,,,,
SYS: @@ Go to the database module to obtain data
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: @@ Switch to the database with slag data
TDB_TCFE10: sw slag4
   ... the command in full is SWITCH_DATABASE
 Current database: Fe-containing Slag  v4.1

 FE                      O  DEFINED
 FEOLIQ  REJECTED
TDB_SLAG4: @@ Some information about the database is given by this command
TDB_SLAG4: d-i
   ... the command in full is DATABASE_INFORMATION
 Current database: Fe-containing Slag  v4.1

                 SLAG4 -- TCS Fe-containing Slag Database
          ****************************************************
                       (Version 4.1, February, 2017)
      Copyright @ 1992-2017: Thermo-Calc Software, Stockholm, Sweden
   This updated SLAG4 Slag Database contains a liquid SLAG phase, as well
     as an Fe-rich liquid phase (dilute solution), a simplified gas phase
     and many stoichiometric solid phases (e.g. oxides, silicates, sulfides,
     halites, etc.), covering the following 30 elements:
         Ag    Al    Ar    B     C     Ca    Co    Cr    Cu    F
         Fe    H     Mg    Mn    Mo    N     Na    Nb    Ni    O
         P     Pb    S     Si    Sn    Ti    U     V     W     Zr
   Thermodynamic data for the liquid SLAG phase and oxide/silicate solid
     phases in the Al2O3-CaO-CrO-Cr2O3-FeO-Fe2O3-MgO-MnO-Na2O-P2O5-SiO2-
     TiO2 system (with extensions to include sulfide/flouride/phosphate
     and postulated oxide/sulfide/flouride/phosphate/silicate compounds)
     were critically assessed by IRSID (1984) and TCS (since 1997),
     using the Kapoor-Frohberg-Gaye Quasichemical Cell Model, i.e., the
     Kapoor-Frohberg Slag Model with the extensions introduced by Gaye
     and Welfringer (1984) for complex multicomponent liquid slag systems.
   Data for the additional components S, 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, Ti+4, P+5, (PO)+3, O-2, S-2 & F-]
     in the liquid SLAG phase and some O-/S-/P-/F-bearing solid phases,
     which were critically assessed by IRSID (1997) and TCS (since 1997),
     have been added to the database, and it thus allows calculations of
     sulfide capacities, phosphorus distribution between the liquid SLAG
     and FE_LIQUID, and many other specific properties of liquid SLAG
     within the framework of 13 elements:
       Al-Ca-Cr-Fe-Mg-Mn-Na-P-Si-Ti-O-S-F
     More elements and in more redox-states will be gradually included in
     future versions of the SLAG database.
   Note that solid solutions are not included in this particular SLAG4
     version, implying that at present all the solid phases are simply
     treated as stoichiometric phases, e.g. the Mg-olivine is modelled as
     the stoichiometric MG2O2_SIO2 phase and the Fe-olivine is modelled as
     another stoichiometric phase FE2O2_SIO2.
   Data for the dilute solution of many elements in the Fe-rich liquid phase
     FE_LIQUID are critically assessed and converted to regular solution
     parameters according to Hillert (1986), with modified dilute solution
     parameters (plus a quadratic term) in Fe-rich liquid from Sigworth
     and Elliot (1974), so that it becomes a consistent thermodynamic model
     and also generally improves the agreements of calculated results with
     available experimental data obtained from steel-making metallurgical
     processes. The following 26 dilute components are included in the
     FE_LIQUID solution phase:
       Ag Al B C Ca Co Cr Cu H Mg Mn Mo N Nb Ni O P Pb S Si Sn Ti U V W Zr
     Thermodynamic data for the FE_LIQUID solution phase are evaluated at
     infinite dilution. The recommended composition limit of any minority
     component, in the 27-component diluted Fe-rich liquid, is only 0.1 wt%,
     i.e. valid in the application of low-alloyed steels. In some cases,
```

```
     the FE_LIQUID data could be used at much higher concentrations e.g.
     in the stainless steel in combination of the liquid SLAG phase, but the
     user must carefully check each of such cases.
   The SLAG4 database is suitable and efficient for various thermodynamic
     calculations in multi-component systems such as chemical activities,
     sulfide capacities, phosphorus distributions, phase equilibria, and
     many other properties in a wide range of metallurgical slag systems,
     especially for (but not limited to) steel-making processes. It can
     be used not only for slag system (liquid slag and solid slag phases)
     but also for alloy-slag-gas heterogeneous interaction processes.
   For steels and various alloys, as well as other substances or solution
     phases, which are in interactions with the Fe-rich FE_LQIUID phase or
     the liquid SLAG phase, thermodynamic data can be appended from other
     available databases, such as TCFE, TCNI, SSOL+SSUB, etc. For more
     information on such databases, please consult Thermo-Calc Software.
   liquid SLAG phase described by Kapoor-Frohberg-Gaye cell model
    Cations in the order of
           P+5, Si+4, Ti+4, (PO)+3, Cr+3, Al+3, Fe+3,
           Cr+2, Fe+2, Mn+2, Mg+2, Ca+2, Na+1
    The name of constituents are A0_kk_CiiCjj_uv_Text
    where kk is the anion index number
          ii is the cation1 index number
          jj is the cation2 index number
          u and v are stoichiometries of cation and anion (when ii=00)
          Text is the normal formula
    Examples: A0_01_C00C07_23_CR2O3  = CR2O3       = Cr2O3
              A0_02_C00C08_23_AL2S3  = AL2S3       = Al2S3
              A0_03_C00C10_23_FE2F6  = FE2F6       = Fe2F6
              A0_01_C07C14_CRCR      = CR3O3CR2O3  = Cr5O6
              A0_01_C07C16_CRFE      = FE3O3CR2O3  = Fe3Cr2O6
              A0_01_C04C10_SIFE      = FE4O12SI3   = Fe4Si3O12
              A0_01_C09C27_BCA       = B2O3CA3O3   = Ca3B2O6
              A0_02_C10C14_FECR      = CR3FE2S6    = Cr3S3.Fe2S3
              A0_03_C08C27_ALCA      = AL2CA3F12   = Ca3F6.Al2F6
    Index for cations and anions:
      Anions  (kk):
        1     2     3
        O-2   S-2  (F2)-2
    ==================================================================
      Cations (ii or jj):
          1     2     3     4     5     6     7     8     9    10
               P+5        Si+4  Ti+4 (PO)+3 Cr+3  Al+3        Fe+3
    ------------------------------------------------------------------
         11    12    13    14    15    16    17    18    19    20
                          Cr+2        Fe+2
    ------------------------------------------------------------------
         21    22    23    24    25    26    27    28    29    30
              Mn+2        Mg+2              Ca+2              Na+1
    Release History:
     Version 1.0-1.1, initial release,          (1992-2001)
              liquid SLAG Al2O3-CaO-FeO-Fe2O3-MgO-MnO-SiO2,
          plus S, F, P2O5, and Na2O, CrO & Cr2O3.
              FE_LIQUID Ag Al B C Ca Co Cr Cu Fe H Mg Mn
                Mo N Nb Ni O P Pb S Si Sn Ti U V W Zr
              GAS phase Ar C1O1 C1O2 N2 O2 O2S1 O3S1 S2
    Version 2.0-2.4, major improvements,        (2002-2008)
              reconstructed the database files
              completed gas phase description covered 30 elements
              corrected the implementation of the FE_LIQUID phase
              added Ti-bearing species, liquid and solid phases
    Version 3.0-3.2, major improvements,       (2009-2015)
              added/corrected many solid phases
              re-arranged references
              default-reject the FEOLIQ phase
              SLAG3param.TDB & SLAG3funct_SEQ.TDB merged
                into the single SLAG3setup.TDB
              phosphorus removed from the liquid SLAG in version 3.2
    Version 4.0-4.1, major improvements,            (2016- )
              phosphorus re-optimized and added back into liquid SLAG
              modified some solid phases e.g. fluorides, Ca-phosphates
              added liquid SLAG constituents for some flourides
    simplified GAS Ar,C1O1,C1O2,H2,H2O1,N2,Na,O2,P2,P4,S2
              more details for database information
   Edited by: Pingfang Shi (Thermo-Calc Software, Sweden), 2002-2010.
             Lina Kjellqvist (Thermo-Calc Software, Sweden), 2012-2013.
             Huahai Mao (Thermo-Calc Software, Sweden), 2015-.
TDB_SLAG4:Hit RETURN to continue
TDB_SLAG4: @@ Define the system by giving the elements. Note that Fe
TDB_SLAG4: @@ and O are included by default.
TDB_SLAG4:
TDB_SLAG4: d-sys mn si cr al
   ... the command in full is DEFINE_SYSTEM
 MN                    SI                    CR
 AL  DEFINED
TDB_SLAG4: @@ 'GET' reads thermodynamic data from the database files to the
TDB_SLAG4: @@ program
TDB_SLAG4: get
   ... the command in full is GET_DATA
14:40:49,043 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 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
 Creating a new composition set SLAG#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'SLAG2 (2006): TCS Fe-Containing Slag Database, V2.3, owned and provided
      by Thermo-Calc Software.'
  'Pingfang Shi (2006), unpublished assessments of CrO/Cr2O3-bearing
      systems. '
  'L Kjellqvist (2013), unpublished work; Fe3O4 stability'
  'TCMP2 (2009): TCS Materials Processing Database, V2.5, owned and provided
      by Thermo-Calc Software.'
 -OK-
14:40:50,969 WARN  The handling of the fraction limits command is not yet supported in GES6.
14:40:51,285 WARN  The handling of the default stable command is not yet supported in GES6.
TDB_SLAG4: go p-3
   ... the command in full is GOTO_MODULE
```

```
 POLY version  3.32
POLY: @@ There are many commands in the POLY-3 module

POLY: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  GOTO_MODULE              REINITIATE_MODULE
 ADVANCED_OPTIONS         HELP                     SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  INFORMATION              SELECT_EQUILIBRIUM
 BACK                     LIST_AXIS_VARIABLE       SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_CONDITIONS          SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_EQUILIBRIUM         SET_CONDITION
 COMPUTE_TRANSITION       LIST_INITIAL_EQUILIBRIA  SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_STATUS              SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_SYMBOLS             SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
 DEFINE_MATERIAL          MACRO_FILE_OPEN          SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MAKE_COMPONENT_ENTERED   SET_START_VALUE
 DELETE_SYMBOL            MAKE_COMPONENT_SUSPENDED SHOW_VALUE
 ENTER_SYMBOL             MAP                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       POST                     TABULATE
 EXIT                     READ_WORKSPACES
POLY:Hit RETURN to continue
POLY: @@ Some basic information is given by the INFORMATION command
POLY: @@ Look at TCEX-01 for more details.
POLY: info
   ... the command in full is INFORMATION
 FILE SYSTEM ERROR                    37
 *** ERROR  1717 IN MLOPEN: FILE DOES NOT EXIST: c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\help\poly3.hlp
POLY: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  GOTO_MODULE              REINITIATE_MODULE
 ADVANCED_OPTIONS         HELP                     SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  INFORMATION              SELECT_EQUILIBRIUM
 BACK                     LIST_AXIS_VARIABLE       SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_CONDITIONS          SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_EQUILIBRIUM         SET_CONDITION
 COMPUTE_TRANSITION       LIST_INITIAL_EQUILIBRIA  SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_STATUS              SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_SYMBOLS             SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
 DEFINE_MATERIAL          MACRO_FILE_OPEN          SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MAKE_COMPONENT_ENTERED   SET_START_VALUE
 DELETE_SYMBOL            MAKE_COMPONENT_SUSPENDED SHOW_VALUE
 ENTER_SYMBOL             MAP                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       POST                     TABULATE
 EXIT                     READ_WORKSPACES
POLY:
POLY:Hit RETURN to continue
POLY: @@ Now set the conditions i.e. the temperature, pressure and
POLY: @@ composition. We are interested in the situation at the
POLY: @@ outflow of steel
POLY:
POLY: s-c t=1800,p=101325,n=1
   ... the command in full is SET_CONDITION
POLY: @@ As conditions you can specify that the steel should have
POLY: @@ 18 weight percent of Cr, 0.4 w/o Mn and 0.4 w/o Si
POLY: @@ (Note that the overall amount of Cr and Mn is not specified).
POLY:
POLY: s-c w(mn)=.004,w(cr)=.18,w(si)=.004
   ... the command in full is SET_CONDITION
POLY: @@ The amount of Al is very small, assume 7 ppm
POLY: s-c w(al)=7e-6
   ... the command in full is SET_CONDITION
POLY: @@ We will later assume that the oxygen potential is determined
POLY: @@ by the equilibrium with liquid slag but initially we assume
POLY: @@ there is 100 ppm O
POLY:
POLY: s-c w(o)=1e-4
   ... the command in full is SET_CONDITION
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6,
    W(O)=1E-4
 DEGREES OF FREEDOM 0
POLY:Hit RETURN to continue
POLY: @@ Check what phases there are
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 SIO2                     ENTERED      0.000000E+00    0.000000E+00
 MNO_SIO2                 ENTERED      0.000000E+00    0.000000E+00
 MNO_AL2O3                ENTERED      0.000000E+00    0.000000E+00
 MNO                      ENTERED      0.000000E+00    0.000000E+00
 MN2O2_SIO2               ENTERED      0.000000E+00    0.000000E+00
 FEO_AL2O3                ENTERED      0.000000E+00    0.000000E+00
 FEO                      ENTERED      0.000000E+00    0.000000E+00
 FE3O4                    ENTERED      0.000000E+00    0.000000E+00
 FE2O3                    ENTERED      0.000000E+00    0.000000E+00
 FE2O2_SIO2               ENTERED      0.000000E+00    0.000000E+00
 CR2O3                    ENTERED      0.000000E+00    0.000000E+00
 AL6O9_SI2O4              ENTERED      0.000000E+00    0.000000E+00
 AL2O3                    ENTERED      0.000000E+00    0.000000E+00
 SLAG#2                   ENTERED      0.000000E+00    0.000000E+00
 SLAG#1                   ENTERED      0.000000E+00    0.000000E+00
 FE_LIQUID                ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
POLY: @@ Start by assuming all other phases except FE_LIQUID are suspended
POLY:
POLY: ch-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY: ch-st p fe-l=ent 0
   ... the command in full is CHANGE_STATUS
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6,
    W(O)=1E-4
 DEGREES OF FREEDOM 0
POLY:Hit RETURN to continue
POLY: @@ The degree of freedom is zero and we can make a calculation.
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
```

```
Calculated          1311 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: @@ Now set the suspended phases as dormant except SLAG#2
POLY: @@ that is not needed in this example
POLY:
POLY: c-st p *s=d
   ... the command in full is CHANGE_STATUS
POLY: c-st p slag#2=sus
   ... the command in full is CHANGE_STATUS
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 FE_LIQUID              ENTERED      0.000000E+00    1.000000E+00
 AL2O3                  DORMANT     -4.467190E-03
 AL6O9_SI2O4            DORMANT     -4.414257E-02
 SLAG#1                 DORMANT     -8.455822E-02
 MNO_AL2O3              DORMANT     -1.635823E-01
 FEO_AL2O3              DORMANT     -4.636329E-01
 CR2O3                  DORMANT     -4.826177E-01
 SIO2                   DORMANT     -4.983783E-01
 MNO_SIO2               DORMANT     -5.733375E-01
 MN2O2_SIO2             DORMANT     -6.753541E-01
 MNO                    DORMANT     -1.454579E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN   -1.526664E+00
 FE2O2_SIO2 FEO FE3O4 FE2O3 GAS
 SUSPENDED PHASES:
 SLAG#2
POLY:Hit RETURN to continue
POLY: @@ If the stable phases do not change in 12 iterations the program
POLY: @@ terminates even if the program has not calculated the correct
POLY: @@ driving forces for the metastable phases.
POLY: @@ You can change this with the command SET-NUMERICAL-LIMITS
POLY: @@ Use this command to change the lowest value of a fraction variable.
POLY:
POLY: s-n-l 500 1E-6 1E-12 n
   ... the command in full is SET_NUMERICAL_LIMITS
 LIMITATIONS of the present version of Thermo-Calc
 Max number of elements                      :  80
 Max number of species                       :5000
 Max number of sublattices in a phase        :  10
 Max number of constituents in a phase:      : 200
 Max number of constituents in an ideal phase :5000
POLY:Hit RETURN to continue
POLY: @@ Calculate again
POLY: 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: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 FE_LIQUID              ENTERED      0.000000E+00    1.000000E+00
 AL2O3                  DORMANT     -4.467190E-03
 AL6O9_SI2O4            DORMANT     -4.414257E-02
 SLAG#1                 DORMANT     -8.455823E-02
 MNO_AL2O3              DORMANT     -1.635823E-01
 FEO_AL2O3              DORMANT     -4.636329E-01
 CR2O3                  DORMANT     -4.826177E-01
 SIO2                   DORMANT     -4.983783E-01
 MNO_SIO2               DORMANT     -5.733375E-01
 MN2O2_SIO2             DORMANT     -6.753541E-01
 MNO                    DORMANT     -1.454579E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN   -1.526664E+00
 FE2O2_SIO2 FEO FE3O4 FE2O3 GAS
 SUSPENDED PHASES:
 SLAG#2
POLY:Hit RETURN to continue
POLY: @@ The driving forces are quite stable.
POLY: @@ Now set the slag phase to stable and let the program
POLY: @@ adjust the amount of oxygen to make it stable
POLY:
POLY: c-st p slag=fix 0
   ... the command in full is CHANGE_STATUS
POLY: s-c w(o)
   ... the command in full is SET_CONDITION
Value /1E-04/: none
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6
 FIXED PHASES
 SLAG#1=0
 DEGREES OF FREEDOM 0
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          406 grid points in              0 s
    84 ITS,  CPU TIME USED   5 SECONDS
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG4

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6
 FIXED PHASES
 SLAG#1=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  5.48785E+01
 Total Gibbs energy -1.12608E+05,  Enthalpy  7.10038E+04,  Volume  0.00000E+00
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```
 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                       1.4237E-05  7.0000E-06 2.0751E-10 -3.3368E+05 SER
 CR                       1.8998E-01  1.8000E-01 5.0828E-04 -1.1351E+05 SER
 FE                       7.9780E-01  8.1188E-01 6.2366E-04 -1.1045E+05 SER
 MN                       3.9957E-03  4.0000E-03 2.3988E-06 -1.9367E+05 SER
 O                        3.9731E-04  1.1583E-04 3.9335E-13 -4.2749E+05 SER
 SI                       7.8161E-03  4.0000E-03 4.4735E-08 -2.5326E+05 SER

 FE_LIQUID                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4879E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.11877E-01  SI  4.00000E-03  O   1.15830E-04
 CR  1.80000E-01  MN  4.00000E-03  AL  7.00000E-06

 SLAG#1                       Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   4.17908E-01  MN  1.47499E-01  CR  6.56802E-02
 AL  2.59239E-01  SI  9.61048E-02  FE  1.35684E-02

 AL2O3                        Status DORMANT     Driving force  7.2947E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 AL  5.29261E-01  SI  0.00000E+00  FE  0.00000E+00
 O   4.70739E-01  MN  0.00000E+00  CR  0.00000E+00

 AL6O9_SI2O4                  Status DORMANT     Driving force  3.8932E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   4.88176E-01  SI  1.31839E-01  FE  0.00000E+00
 AL  3.79984E-01  MN  0.00000E+00  CR  0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ List the status of the phases.
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 SLAG#1                   FIXED        0.000000E+00    0.000000E+00
 FE_LIQUID                ENTERED      0.000000E+00    1.000000E+00
 AL2O3                    DORMANT      7.294695E-02
 AL6O9_SI2O4              DORMANT      3.893195E-02
 MNO_AL2O3                DORMANT     -8.744049E-02
 FEO_AL2O3                DORMANT     -3.874379E-01
 CR2O3                    DORMANT     -3.950177E-01
 SIO2                     DORMANT     -4.011528E-01
 MNO_SIO2                 DORMANT     -4.858179E-01
 MN2O2_SIO2               DORMANT     -5.919941E-01
 MNO                      DORMANT     -1.381619E+00
 FE2O2_SIO2               DORMANT     -1.443198E+00
 FEO                      DORMANT     -2.363396E+00
 FE3O4                    DORMANT     -3.110318E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN   -3.826291E+00
 FE2O3 GAS
 SUSPENDED PHASES:
 SLAG#2
POLY:Hit RETURN to continue
POLY: @@ Note that mullite and corundum are stable.
POLY: @@ The amount of Al is probably too high, set it
POLY: @@ to half of the initial value
POLY:
POLY: s-c w(al)=3.5e-6
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    78 ITS,  CPU TIME USED   4 SECONDS
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 SLAG#1                   FIXED        0.000000E+00    0.000000E+00
 FE_LIQUID                ENTERED      0.000000E+00    1.000000E+00
 AL6O9_SI2O4              DORMANT     -3.253602E-02
 AL2O3                    DORMANT     -8.735188E-02
 MNO_AL2O3                DORMANT     -1.696491E-01
 SIO2                     DORMANT     -2.505437E-01
 CR2O3                    DORMANT     -2.592749E-01
 MNO_SIO2                 DORMANT     -3.502456E-01
 MN2O2_SIO2               DORMANT     -4.628662E-01
 FEO_AL2O3                DORMANT     -4.695392E-01
 MNO                      DORMANT     -1.268602E+00
 FE2O2_SIO2               DORMANT     -1.313855E+00
 DORMANT PHASES WITH DRIVING FORCE LESS THAN   -2.250003E+00
 FEO FE3O4 FE2O3 GAS
 SUSPENDED PHASES:
 SLAG#2
POLY: @@ Now the Al2O3 phases are not stable.
POLY: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG4

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=3.5E-6
 FIXED PHASES
 SLAG#1=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  5.48748E+01
 Total Gibbs energy -1.12638E+05,  Enthalpy  7.09855E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                       7.1181E-06  3.5000E-06 9.8926E-11 -3.4477E+05 SER
 CR                       1.8997E-01  1.8000E-01 5.0791E-04 -1.1352E+05 SER
 FE                       7.9772E-01  8.1185E-01 6.2370E-04 -1.1045E+05 SER
 MN                       3.9954E-03  4.0000E-03 2.3972E-06 -1.9368E+05 SER
 O                        4.9733E-04  1.4500E-04 4.9345E-13 -4.2410E+05 SER
 SI                       7.8155E-03  4.0000E-03 4.4663E-08 -2.5329E+05 SER

 FE_LIQUID                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4875E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.11852E-01  SI  4.00000E-03  O   1.44998E-04
 CR  1.80000E-01  MN  4.00000E-03  AL  3.50000E-06

 SLAG#1                       Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   4.16763E-01  AL  1.75458E-01  CR  6.11817E-02
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 MN  1.79792E-01  SI  1.54667E-01  FE  1.21379E-02
POLY:Hit RETURN to continue
POLY: @@ We assume that this describes the situation at 18 w/o Cr. Some
POLY: @@ liquid slag that later will form mainly SiO2-Al2O3-MnO is present.
POLY: @@ Now increase the Cr-content to 25 w/o
POLY:
POLY: s-c w(cr)=.25
   ... the command in full is SET_CONDITION
POLY: 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
    75 ITS,  CPU TIME USED   5 SECONDS
POLY: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG4

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=3.5E-6
 FIXED PHASES
 SLAG#1=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  5.45799E+01
 Total Gibbs energy -1.12759E+05,  Enthalpy  7.08334E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                       7.0799E-06  3.5000E-06 8.0484E-11 -3.4786E+05 SER
 CR                       2.6242E-01  2.5000E-01 6.9398E-04 -1.0885E+05 SER
 FE                       7.2490E-01  7.4173E-01 5.6875E-04 -1.1183E+05 SER
 MN                       3.9739E-03  4.0000E-03 2.5531E-06 -1.9274E+05 SER
 O                        9.2470E-04  2.7106E-04 5.0610E-13 -4.2372E+05 SER
 SI                       7.7735E-03  4.0000E-03 4.4251E-08 -2.5343E+05 SER

 FE_LIQUID                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.4580E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  7.41725E-01  MN  4.00000E-03  O   2.71057E-04
 CR  2.50000E-01  SI  4.00000E-03  AL  3.50000E-06

 SLAG#1                       Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   4.01215E-01  AL  1.48638E-01  CR  8.70498E-02
 MN  2.07286E-01  SI  1.44714E-01  FE  1.10974E-02
POLY:Hit RETURN to continue
POLY: @@ Now Cr2O3 would like to be stable. The simplest correction is to modify
POLY: @@ the composition of the steel in order to decrease the oxygen potential.
POLY: @@ For example the Mn or Si content could be changed.
POLY: @@ In order to determine which of these has the largest influence
POLY: @@ on the oxygen potential, calculate this by the partial derivative
POLY: @@ of the oxygen activity w.r.t. the Mn and Si content.
POLY:
POLY: s-ref-s o gas
   ... the command in full is SET_REFERENCE_STATE
Temperature /*/:
Pressure /1E5/:
POLY: show acr(o)
   ... the command in full is SHOW_VALUE
 ACR(O)=7.413591E-7
POLY: show acr(o).w(mn)
   ... the command in full is SHOW_VALUE
 ACR(O).W(MN)=-3.3090052E-5
POLY: show acr(o).w(si)
   ... the command in full is SHOW_VALUE
 ACR(O).W(SI)=-4.7881618E-5
POLY:Hit RETURN to continue
POLY: @@ The value is largest for Si and thus the smallest change is necessary
POLY: @@ for that. Instead of modifying this content in steps one may
POLY: @@ specify that the Cr2O3 phase should be on its limit of stability, i.e.
POLY: @@ use the command FIX with zero amount and calculate the change
POLY: @@ in composition.
POLY:
POLY: c-s p cr2o3=fix 0
   ... the command in full is CHANGE_STATUS
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=3.5E-6
 FIXED PHASES
 SLAG#1=0    CR2O3=0
 DEGREES OF FREEDOM -1
POLY: s-c w(si)=none
   ... the command in full is SET_CONDITION
POLY: 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
    93 ITS,  CPU TIME USED   4 SECONDS
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG4

 Conditions:
 T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(AL)=3.5E-6
 FIXED PHASES
 SLAG#1=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  5.47614E+01
 Total Gibbs energy -1.11748E+05,  Enthalpy  7.15874E+04,  Volume  0.00000E+00

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                       7.1034E-06  3.5000E-06 7.3699E-11 -3.4917E+05 SER
 CR                       2.6330E-01  2.5000E-01 6.9619E-04 -1.0880E+05 SER
 FE                       7.3071E-01  7.4519E-01 5.7374E-04 -1.1170E+05 SER
 MN                       3.9871E-03  4.0000E-03 2.4318E-06 -1.9346E+05 SER
 O                        1.0148E-03  2.9650E-04 9.0243E-07 -2.0830E+05 GAS
 SI                       9.8588E-04  5.0562E-04 5.1341E-09 -2.8566E+05 SER

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

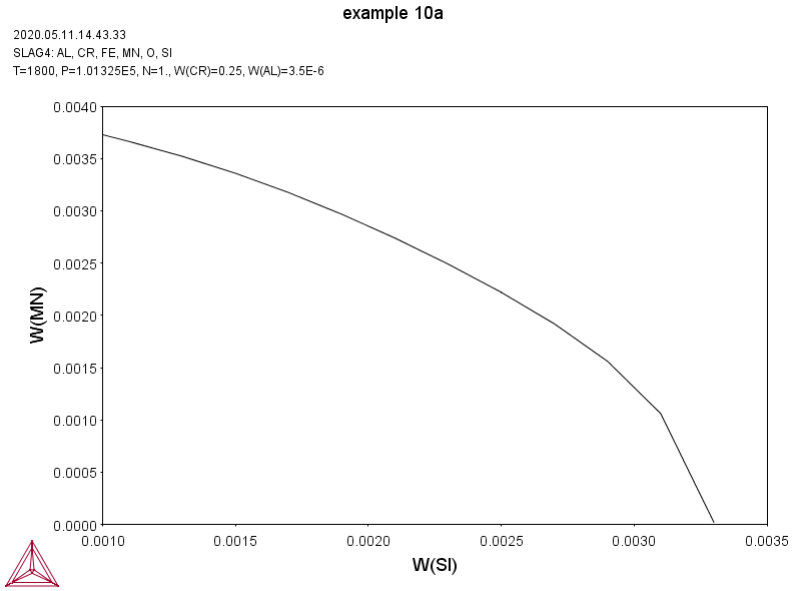
```
 Moles 1.0000E+00, Mass 5.4761E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  7.45194E-01  MN  4.00000E-03  O   2.96496E-04
 CR  2.50000E-01  SI  5.05622E-04  AL  3.50000E-06

 SLAG#1                     Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 O   3.49148E-01  MN  1.94532E-01  FE  1.77668E-02
 CR  2.47028E-01  AL  1.85879E-01  SI  5.64632E-03

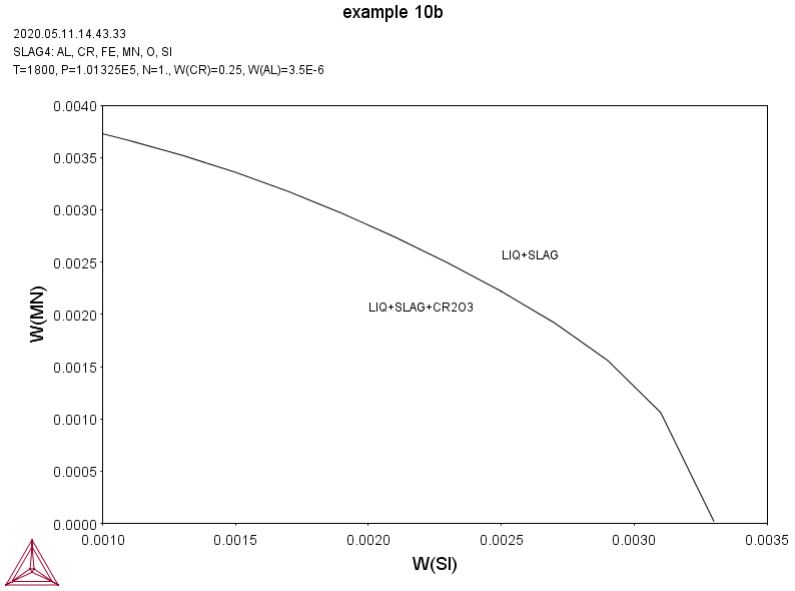
 CR2O3                      Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CR  6.84207E-01  AL  0.00000E+00  FE  0.00000E+00
 O   3.15793E-01  MN  0.00000E+00  SI  0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ We can read the new Si content from this list but also
POLY: @@ directly show the value of a variable
POLY: sh w(si)
   ... the command in full is SHOW_VALUE
 W(SI)=5.0562165E-4
POLY: @@ Increase the Si content to 0.3 w/o to avoid forming Cr2O3.
POLY: @@ Calculate also how much the Mn content must be changed
POLY: s-c w(si)=.003
   ... the command in full is SET_CONDITION
POLY: s-c w(mn)=none
   ... the command in full is SET_CONDITION
POLY: 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
   148 ITS,  CPU TIME USED   7 SECONDS
POLY: sh w(mn)
   ... the command in full is SHOW_VALUE
 W(MN)=1.3395362E-3
POLY: @@ Check with Si content equal to 0.25. It should be consistent with
POLY: @@ the plot below, i.e. Mn content decreases with increasing Si content.
POLY: s-c w(si)=.0025
   ... the command in full is SET_CONDITION
POLY: 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
   118 ITS,  CPU TIME USED   5 SECONDS
POLY: sh w(mn)
   ... the command in full is SHOW_VALUE
 W(MN)=2.2202683E-3
POLY:Hit RETURN to continue
POLY: @@ Plot how the Mn content varies when the Si content
POLY: @@ varies between 0.1 and 0.4 w/o.
POLY: s-a-v 1 w(si) 0.001 0.004 0.0002
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex10 y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.250000E-02
...OK

 Phase Region from   0.250000E-02 for:
     FE_LIQUID
     SLAG#1
     CR2O3
 QBSMER trying to find equilibrium at   3.3400000E-03
 QBSMER: Second global calculation
 Calculated     7 equilibria
 Sorry cannot continue  1717  55 1    3.3000000E-03

 Phase Region from   0.250000E-02 for:
     FE_LIQUID
     SLAG#1
     CR2O3
 Global test at  1.00000E-03 .... OK
 Terminating at   0.100000E-02
 Calculated    11 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex10\tcex10.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x w(si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(mn)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 10a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:Hit RETURN to continue
POST: add .0025 .0025 n
   ... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG
Text size: /.36/:
POST: add .002 .002 n
   ... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG+CR2O3
Text size: /.36/:
POST: set-title example 10b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex11

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex11\tcex11.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Oxidation of Cu2S with an H2O/O2 gas mixture
SYS:
SYS: @@ This example demonstrates the oxidation of Cu2S
SYS: @@ with an H2O/O2 gas mixture. Thermo-Calc is used to find
SYS: @@ the optimum O/H ratio (i.e. oxygen potential) as certain
SYS: @@ oxygen potential values can desulphurize Cu2S without
SYS: @@ forming copper oxides.
SYS:
SYS: @@ In Thermo-Calc, the problem reduces to perform equilibria
SYS: @@ calculations in a Cu-S-H-O system. The amounts of the
SYS: @@ components should be kept to correct ratio corresponding
SYS: @@ to Cu2S and H2O using a command SET_INPUT_AMOUNTS in POLY3.
SYS:
SYS: @@ Initially, O/H = 0.5 is given. Optimum O/H ratio is
SYS: @@ calculated with the desired calculation conditions. For
SYS: @@ example, to simulate one phase disappearing, you can FIX
SYS: @@ the phase with zero amount.
SYS:
SYS: set-log ex11,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw
   ... the command in full is SWITCH_DATABASE
 Use one of these databases

 TCFE10  =  Steels/Fe-Alloys  v10.1
 TCFE9   =  Steels/Fe-Alloys  v9.2
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.2
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.1
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX10  =  Metal Oxide Solutions  v10.0
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
```

```
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.3
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v3.0
 ALDEMO  =  Aluminum Demo Database v4.0
 NIDEMO  =  Nickel Demo Database v2.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v3.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE10/: user tcex11.tdb
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
14:44:51,229 INFO  USER_1377915951_11, number of lines read: 547
14:44:51,987 INFO  Parsing of USER_1377915951_11 completed in 892 ms
TDB_USER: def-sys cu s o h
   ... the command in full is DEFINE_SYSTEM
 CU                      S                       O
 H  DEFINED
TDB_USER: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 GAS:G       :CU CU1H1 CU1H1O1 CU1O1 CU1S1 CU2 CU2S1 H H1O1 H1O1S1_HSO
  H1O1S1_SOH H1O2 H1S1 H2 H2O1 H2O1S1_H2SO H2O1S1_HSOH H2O2 H2O4S1 H2S1 H2S2
  O O1S1 O1S2 O2 O2S1 O3 O3S1 S S2 S3 S4 S5 S6 S7 S8:
 CU          :CU:
 CU2O        :CU2O1:
 CU2O_L      :CU2O1:
 CU2S        :CU2S1:
 CU2SO4      :CU2O4S1:
 CU2SO5      :CU2O5S1:
 CU2S_L      :CU2S1:
 CU2S_S2     :CU2S1:
 CU2S_S3     :CU2S1:
 CUO         :CU1O1:
 CUS         :CU1S1:
 CUSO4       :CU1O4S1:
 CU_L        :CU:
 H2O2_L      :H2O2:
 H2O_L       :H2O1:
 H2SO4_L     :H2O4S1:
 S           :S:
 S_L         :S:
 S_S2        :S:
TDB_USER:Hit RETURN to continue
TDB_USER: get
   ... the command in full is GET_DATA
14:44:52,268 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
```

```
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

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

 POLY version  3.32
POLY: ?
   ... the command in full is HELP
 ADD_INITIAL_EQUILIBRIUM  GOTO_MODULE              REINITIATE_MODULE
 ADVANCED_OPTIONS         HELP                     SAVE_WORKSPACES
 AMEND_STORED_EQUILIBRIA  INFORMATION              SELECT_EQUILIBRIUM
 BACK                     LIST_AXIS_VARIABLE       SET_ALL_START_VALUES
 CHANGE_STATUS            LIST_CONDITIONS          SET_AXIS_VARIABLE
 COMPUTE_EQUILIBRIUM      LIST_EQUILIBRIUM         SET_CONDITION
 COMPUTE_TRANSITION       LIST_INITIAL_EQUILIBRIA  SET_INPUT_AMOUNTS
 CREATE_NEW_EQUILIBRIUM   LIST_STATUS              SET_INTERACTIVE
 DEFINE_COMPONENTS        LIST_SYMBOLS             SET_NUMERICAL_LIMITS
 DEFINE_DIAGRAM           LOAD_INITIAL_EQUILIBRIUM SET_REFERENCE_STATE
 DEFINE_MATERIAL          MACRO_FILE_OPEN          SET_START_CONSTITUTION
 DELETE_INITIAL_EQUILIB   MAKE_COMPONENT_ENTERED   SET_START_VALUE
 DELETE_SYMBOL            MAKE_COMPONENT_SUSPENDED SHOW_VALUE
 ENTER_SYMBOL             MAP                      STEP_WITH_OPTIONS
 EVALUATE_FUNCTIONS       POST                     TABULATE
 EXIT                     READ_WORKSPACES
POLY: li-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 CU                       ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 S                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 S_S2                     ENTERED      0.000000E+00    0.000000E+00
 S_L                      ENTERED      0.000000E+00    0.000000E+00
 S                        ENTERED      0.000000E+00    0.000000E+00
 H2SO4_L                  ENTERED      0.000000E+00    0.000000E+00
 H2O_L                    ENTERED      0.000000E+00    0.000000E+00
 H2O2_L                   ENTERED      0.000000E+00    0.000000E+00
 CU_L                     ENTERED      0.000000E+00    0.000000E+00
 CUSO4                    ENTERED      0.000000E+00    0.000000E+00
 CUS                      ENTERED      0.000000E+00    0.000000E+00
 CUO                      ENTERED      0.000000E+00    0.000000E+00
 CU2S_S3                  ENTERED      0.000000E+00    0.000000E+00
 CU2S_S2                  ENTERED      0.000000E+00    0.000000E+00
 CU2S_L                   ENTERED      0.000000E+00    0.000000E+00
 CU2SO5                   ENTERED      0.000000E+00    0.000000E+00
 CU2SO4                   ENTERED      0.000000E+00    0.000000E+00
 CU2S                     ENTERED      0.000000E+00    0.000000E+00
 CU2O_L                   ENTERED      0.000000E+00    0.000000E+00
 CU2O                     ENTERED      0.000000E+00    0.000000E+00
 CU                       ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CU          ENTERED    H15O10.5S1  ENTERED    O           ENTERED
 CU1H1       ENTERED    H1O1        ENTERED    O1S1        ENTERED
 CU1H10O9S1  ENTERED    H1O1S1_HSO  ENTERED    O1S2        ENTERED
 CU1H1O1     ENTERED    H1O1S1_SOH  ENTERED    O2          ENTERED
 CU1H2O2     ENTERED    H1O2        ENTERED    O2S1        ENTERED
 CU1H2O5S1   ENTERED    H1S1        ENTERED    O3          ENTERED
 CU1H6O7S1   ENTERED    H2          ENTERED    O3S1        ENTERED
 CU1O1       ENTERED    H2O1        ENTERED    S           ENTERED
 CU1O4S1     ENTERED    H2O1S1_H2SO ENTERED    S2          ENTERED
 CU1S1       ENTERED    H2O1S1_HSOH ENTERED    S3          ENTERED
 CU2         ENTERED    H2O2        ENTERED    S4          ENTERED
 CU2O1       ENTERED    H2O4S1      ENTERED    S5          ENTERED
 CU2O4S1     ENTERED    H2S1        ENTERED    S6          ENTERED
 CU2O5S1     ENTERED    H2S2        ENTERED    S7          ENTERED
 CU2S1       ENTERED    H4O5S1      ENTERED    S8          ENTERED
 H           ENTERED    H6O6S1      ENTERED    VA          ENTERED
 H10O8S1     ENTERED    H8O7S1      ENTERED
POLY:

POLY:Hit RETURN to continue
POLY: @@ Assume initially that we have one mole of Cu2S and 50 moles water vapor
POLY: s-i-a n(cu2s1)=1,n(h2o1)=50
   ... the command in full is SET_INPUT_AMOUNTS
POLY: set-cond t=1400,p=101325
   ... the command in full is SET_CONDITION
POLY: 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: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
14:44:53,398 INFO  Preparing system for use: USER_1377915951_11
14:44:55,181 INFO  Preparing phase for use: GAS
 Using global minimization procedure
14:44:55,654 INFO  Preparing phase for use: CU
14:44:55,776 INFO  Preparing phase for use: CU2O
14:44:56,022 INFO  Preparing phase for use: CU2O_L
14:44:56,491 INFO  Preparing phase for use: CU2S
14:44:56,836 INFO  Preparing phase for use: CU2SO4
14:44:56,974 INFO  Preparing phase for use: CU2SO5
14:44:57,107 INFO  Preparing phase for use: CU2S_L
14:44:57,200 INFO  Preparing phase for use: CU2S_S2
14:44:57,344 INFO  Preparing phase for use: CU2S_S3
14:44:57,441 INFO  Preparing phase for use: CUO
14:44:57,567 INFO  Preparing phase for use: CUS
14:44:57,660 INFO  Preparing phase for use: CUSO4
14:44:57,820 INFO  Preparing phase for use: CU_L
14:44:57,908 INFO  Preparing phase for use: H2O2_L
14:44:58,000 INFO  Preparing phase for use: H2O_L
14:44:58,097 INFO  Preparing phase for use: H2SO4_L
14:44:58,188 INFO  Preparing phase for use: S
14:44:58,280 INFO  Preparing phase for use: S_L
```

```
14:44:58,383 INFO  Preparing phase for use: S_S2
Calculated           685 grid points in             2 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     3  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

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

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

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

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

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

 CU_L                         Status ENTERED     Driving force  0.0000E+00
 Moles 4.4883E-01, Mass 2.8522E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  1.00000E+00  S   0.00000E+00  O   0.00000E+00  H   0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Now set the status of the diginite (CU2S_S3) to be fixed with
POLY: @@ zero amount. This means that this is reduced completely
POLY: 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 mole formula units /0/: 0
POLY: @@ There are now too many conditions. The gas must be allowed to vary
POLY: @@ in composition to find the correct oxygen potential
POLY: 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:Hit RETURN to continue
POLY: set-c n(o)=none
   ... the command in full is SET_CONDITION
POLY: 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: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
    10 ITS,  CPU TIME USED   0 SECONDS
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

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

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

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

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

```
 O3S1          1.32878E-07  H2S2          8.37427E-11  S8            1.00000E-30
 CU1H1         5.52244E-08  H1O1S1_HSO    4.83886E-11  S7            1.00000E-30

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

 CU2S_S3                    Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CU  7.98557E-01  S   2.01443E-01  O   0.00000E+00  H   0.00000E+00
POLY: sh n(*)
   ... the command in full is SHOW_VALUE
 N(CU)=2, N(H)=100., N(O)=51.784749, N(S)=1.
POLY:Hit RETURN to continue
POLY: @@ If we have too much oxygen we may get some copper oxides,
POLY: @@ check which one is the closest to be stable
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                  STATUS    DRIVING FORCE   MOLES
 CU2S_S3                FIXED        0.000000E+00    0.000000E+00
 CU_L                   ENTERED      0.000000E+00    1.999928E+00
 GAS                    ENTERED      0.000000E+00    1.527848E+02
 CU2S_L                 ENTERED     -3.931114E-04    0.000000E+00
 CU2S_S2                ENTERED     -3.309936E-02    0.000000E+00
 CU                     ENTERED     -3.549960E-02    0.000000E+00
 CU2S                   ENTERED     -3.332974E-01    0.000000E+00
 CU2O                   ENTERED     -1.086153E+00    0.000000E+00
 CU2O_L                 ENTERED     -1.231036E+00    0.000000E+00
 H2O_L                  ENTERED     -1.738865E+00    0.000000E+00
 CUS                    ENTERED     -3.173417E+00    0.000000E+00
 CUO                    ENTERED     -3.229722E+00    0.000000E+00
 CU2SO4                 ENTERED     -3.322206E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -3.797595E+00
 CU2SO5 CUSO4 H2SO4_L H2O2_L S_L S_S2 S
POLY: @@ Set Cu2O to fix with zero amount and remove the fix status of CU2S_S3
POLY: c-s p cu2o=fix 0
   ... the command in full is CHANGE_STATUS
POLY: c-s p cu2s_s3
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/:
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
    39 ITS,  CPU TIME USED   0 SECONDS
POLY: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

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

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

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

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

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

 CU2O                       Status FIXED       Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CU  8.88190E-01  O   1.11810E-01  S   0.00000E+00  H   0.00000E+00
POLY: show n(*)
   ... the command in full is SHOW_VALUE
 N(CU)=2, N(H)=100., N(O)=51.992866, N(S)=1.
POLY:Hit RETURN to continue
POLY: @@ The ratio N(O) to N(H) should thus be between 0.5178 and 0.52
POLY: @@ in order to reduce all Cu2S and not forming any Cu2O
POLY: @@ Make a diagram showing this amount of phases
POLY: c-st p cu2o
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/:
POLY: 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: s-c n(o)
   ... the command in full is SET_CONDITION
Value /51.99286556/:
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Found the set of lowest grid points in              0 s
```

```
 Calculated POLY solution       0 s, total time     0  s
POLY: save tcex11 y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    51.9929
...OK

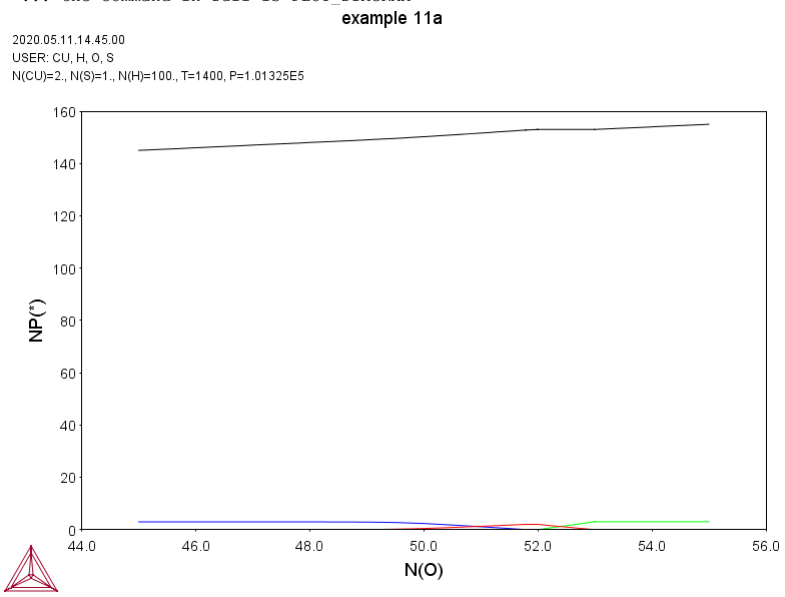
 Phase Region from    51.9929     for:
     GAS
     CU_L
 Global check of adding phase at  5.19929E+01
 Calculated     2 equilibria

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

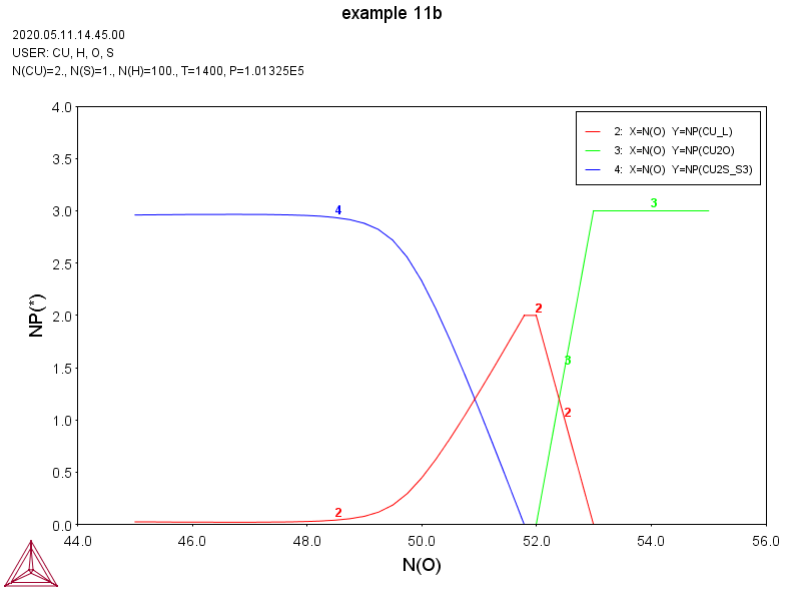
 Phase Region from    52.9928     for:
     GAS
     CU2O
 Global test at  5.49929E+01 .... OK
 Terminating at    55.0000
 Calculated    12 equilibria

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

 Phase Region from    51.7847     for:
     GAS
     CU2S_S3
     CU_L
 Global test at  4.99929E+01 .... OK
 Global test at  4.74929E+01 .... OK
 Global test at  4.50000E+01 .... OK
 Terminating at    45.0000
 Calculated    31 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex11\tcex11.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 11a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s y n 0 4
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 11b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex12

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex12\tcex12.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Tabulation of thermodynamic data for reactions
SYS:
SYS: @@ This example shows a number of independent cases using
SYS: @@ the TABULATE_REACTION (TAB) module to tabulate thermodynamic
SYS: @@ data for reactions.
SYS:
SYS: @@ Note that a SSUB database license is required to run
SYS: @@ the example.
SYS:
SYS: @@ Each case is separated by a line such as this
SYS: @@ ============================
SYS: set-log ex12,,
SYS: go tab
   ... the command in full is GOTO_MODULE
TAB: ?
   ... the command in full is HELP
 BACK                     LIST_SUBSTANCES          SWITCH_DATABASE
 ENTER_FUNCTION           MACRO_FILE_OPEN          TABULATE_DERIVATIVES
 ENTER_REACTION           PATCH                    TABULATE_REACTION
 EXIT                     SET_ENERGY_UNIT          TABULATE_SUBSTANCE
 GOTO_MODULE              SET_INTERACTIVE
 HELP                     SET_PLOT_FORMAT
TAB: @@ Tabulate data for a reaction
TAB: tab-rea 3H2+N2=2N1H3;
   ... the command in full is TABULATE_REACTION
 Use one of these databases

 TCFE10  =  Steels/Fe-Alloys  v10.1
 TCFE9   =  Steels/Fe-Alloys  v9.2
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.2
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.1
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX10  =  Metal Oxide Solutions  v10.0
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
```

```
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
 TCSLD3  =  Solder Alloys  v3.3
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v3.0
 ALDEMO  =  Aluminum Demo Database v4.0
 NIDEMO  =  Nickel Demo Database v2.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v3.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE10/: SSUB6
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: SGTE Substances Database v6.0

 VA  DEFINED
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES .....
   ... the command in full is DEFINE_SPECIES
 H2                      N2                      H3N1
   DEFINED
   ... the command in full is GET_DATA
14:46:18,677 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      H2<G> H2<G>
      HYDROGEN<G>
      STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   H3N1<G> T.C.R.A.S. Class: 2
      H3N1<G> NH3<G>
      AMMONIA <GAS>
   N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      N2<G> N2<G>
      NITROGEN <DIATOMIC GAS>
      PUBLISHED BY JANAF AT 09/65
 -OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /SCREEN/:

               O U T P U T  F R O M  T H E R M O - C A L C
               2020. 5.11                          14.46.21


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

```
 H3N1<GAS>

 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04
  800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02   7.72568E+04
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05
 1100.00  -7.77802E+00  -1.11169E+05  -2.34908E+02   1.47229E+05
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05
TAB:Hit RETURN to continue
TAB: @@ Add a final column with a function. In this function
TAB: @@ you may use G, S, H, V, CP, T and R with the 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:
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
               2020. 5.11                          14.46.21


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

 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04   1.98115E+02
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04   1.98116E+02
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04   1.99799E+02
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03   2.02800E+02
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04   2.05930E+02
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04   2.08834E+02
  800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02   7.72568E+04   2.11421E+02
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05   2.13687E+02
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05   2.15659E+02
 1100.00  -7.77802E+00  -1.11169E+05  -2.34908E+02   1.47229E+05   2.17372E+02
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05   2.18858E+02
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05   2.20149E+02
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05   2.21272E+02
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05   2.22251E+02
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05   2.23107E+02
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05   2.23857E+02
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05   2.24515E+02
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05   2.25093E+02
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05   2.25602E+02
TAB:Hit RETURN to continue
TAB: t-r
   ... the command in full is TABULATE_REACTION
Same reaction? /Y/: y
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /SCREEN/: tcex12a
Grapical output? /Y/: y
Plot column? /2/: 6

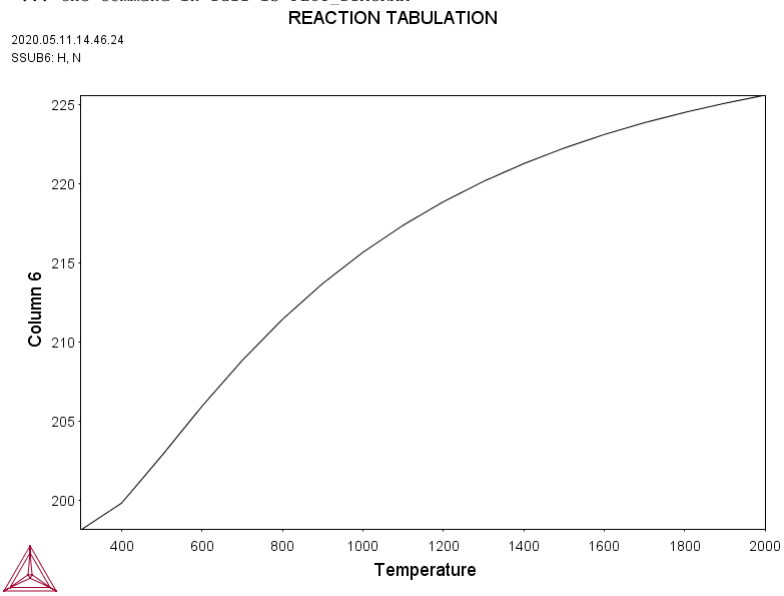
               O U T P U T   F R O M   T H E R M O - C A L C
               2020. 5.11                          14.46.21


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

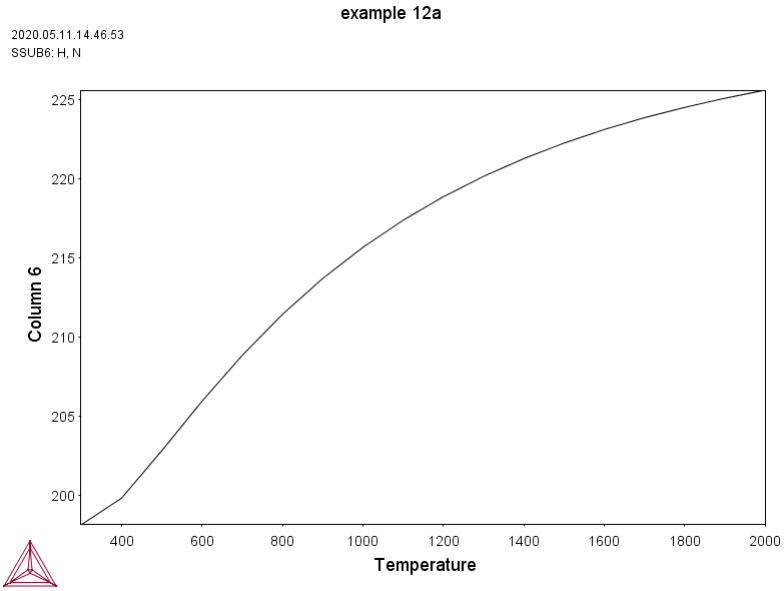
 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04   1.98115E+02
  300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04   1.98116E+02
  400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04   1.99799E+02
  500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03   2.02800E+02
  600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04   2.05930E+02
  700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04   2.08834E+02
```

```
  800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02   7.72568E+04   2.11421E+02
  900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05   2.13687E+02
 1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05   2.15659E+02
 1100.00  -7.77802E+00  -1.11169E+05  -2.34908E+02   1.47229E+05   2.17372E+02
 1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05   2.18858E+02
 1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05   2.20149E+02
 1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05   2.21272E+02
 1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05   2.22251E+02
 1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05   2.23107E+02
 1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05   2.23857E+02
 1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05   2.24515E+02
 1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05   2.25093E+02
 2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05   2.25602E+02

 POSTPROCESSOR VERSION 3.2
  ... the command in full is QUICK_EXPERIMENTAL_PLOT
  ... the command in full is SET_SCALING_STATUS
  ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-title example 12a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 *** ERROR  3004 IN LPOSTP:  NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ In the Gibbs-Enery-System list the data using
TAB: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
GES: l-d
   ... the command in full is LIST_DATA
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?: ?
 FILE SYSTEM ERROR IN FILHLP
 ERROR                    1717  READING HELP FILE
OPTIONS?: rs

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: SSUB6
```

```
 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) = +F11937T+R*T*LN(1E-05*P)
           REFERENCE:10162
      G(GAS,H3N1;0)- 3 H298(1/2_MOLE_H2(GAS),H;0)-H298(1/2_MOLE_N2(GAS),N;0)
           = +F12196T+R*T*LN(1E-05*P)
           REFERENCE:10361
      G(GAS,N2;0)- 2 H298(1/2_MOLE_N2(GAS),N;0) = +F14172T+R*T*LN(1E-05*P)
           REFERENCE:12120

 LIST_OF_REFERENCES
 NUMBER  SOURCE
   REF10162  H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
           H2<G> H2<G>
           HYDROGEN<G>
           STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   REF10361  H3N1<G> T.C.R.A.S. Class: 2
           H3N1<G> NH3<G>
           AMMONIA <GAS>
   REF12120  N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
           N2<G> N2<G>
           NITROGEN <DIATOMIC GAS>
           PUBLISHED BY JANAF AT 09/65

GES:Hit RETURN to continue
GES: back
TAB:
TAB: @@ Tabulate another reaction
TAB: @@ ==============================================
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 GES .....
   ... the command in full is DEFINE_SPECIES
 GA                      IN1P1                   IN
 GA1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   GA1<G> T.C.R.A.S. Class: 1
      GA1<G> Ga<G>
      GALLIUM <GAS>
   GA1P1<G> S.G.T.E.
      GA1P1<G> GaP<G>
      GALLIUM PHOSPHIDE <GAS>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
      from T.C.R.A.S.
   IN1<G> THERMODATA
      IN1<G>
      New Assessment (H_form and S only)
   IN1P1<G> CHATILLON(1994 March)
      IN1P1<G>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   GA1P1 S.G.T.E.
      GA1P1 GaP GAP
      GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
   GA1 S.G.T.E. **
      GA1 Ga
      GALLIUM
      Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
      20080211 BC Tref 200 -> 298.15
   IN1P1 I. BARIN 3rd. Edition
      IN1P1 INP InP
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
   IN1 S.G.T.E. **
      IN1 In
      INDIUM
      Data from SGTE Unary DB
 -OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

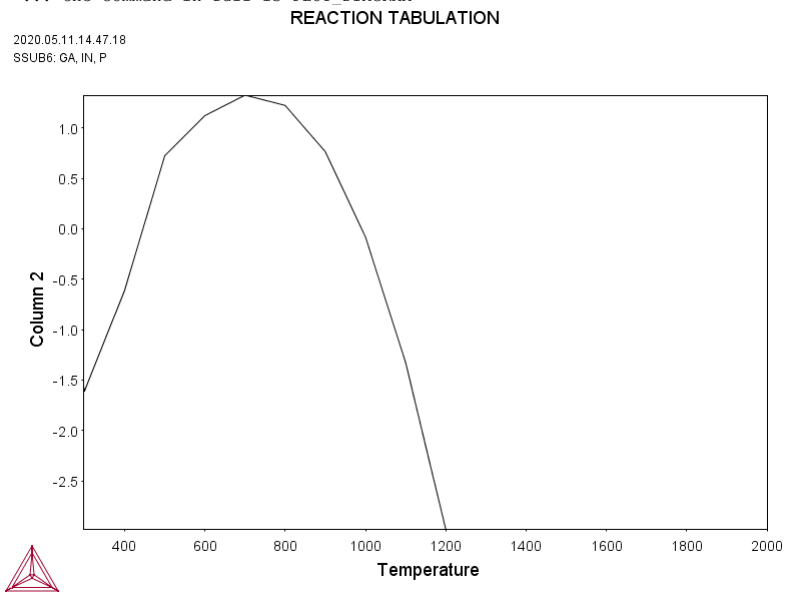
Output file /tcex12a/: tcex12b
Grapical output? /Y/: Y
Plot column? /2/: 2

               O U T P U T  F R O M  T H E R M O - C A L C
               2020. 5.11                          14.47.15
```

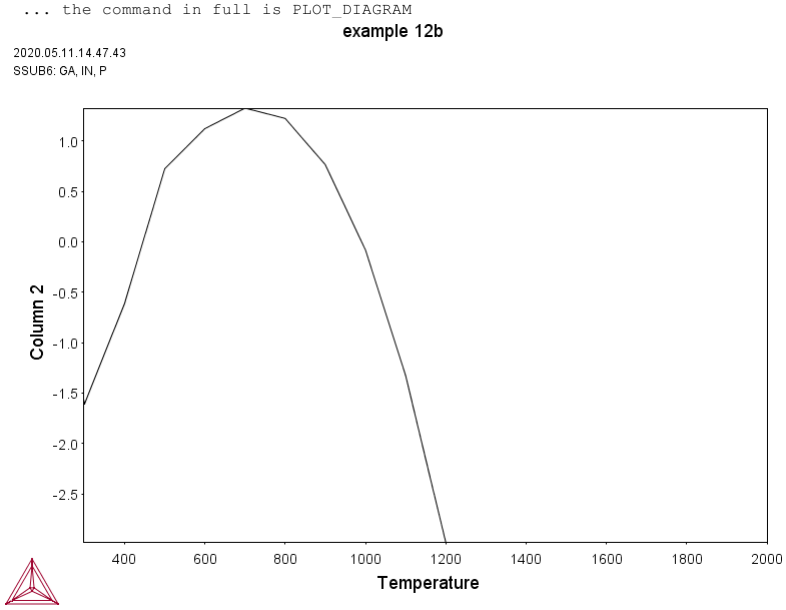
```
Column 6: fef       (G-H298 )/T
Reaction:  GA+IN1P1=IN+GA1P1
GA stable as GA_S
IN1P1 stable as IN1P1_S
IN stable as IN_S
GA1P1 stable as GA1P1_S

*******************************************************************************
   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
Temperature range exceeded for IN1P1

  ... the command in full is QUICK_EXPERIMENTAL_PLOT
  ... the command in full is SET_SCALING_STATUS
  ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-title example 12b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 *** ERROR  3004 IN LPOSTP:  NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ By default a species in a gas is not included in
TAB: @@ a tabulation, you must specify <GAS> if you want that
```

```
TAB: t-r n
   ... the command in full is TABULATE_REACTION
Reaction: INP<gas>+GA=GAP+IN;
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES .....
   ... the command in full is DEFINE_SPECIES
 GA                      IN1P1                   IN
 GA1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   GA1<G> T.C.R.A.S. Class: 1
      GA1<G> Ga<G>
      GALLIUM <GAS>
   GA1P1<G> S.G.T.E.
      GA1P1<G> GaP<G>
      GALLIUM PHOSPHIDE <GAS>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
      from T.C.R.A.S.
   IN1<G> THERMODATA
      IN1<G>
      New Assessment (H_form and S only)
   IN1P1<G> CHATILLON(1994 March)
      IN1P1<G>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   GA1P1 S.G.T.E.
      GA1P1 GaP GAP
      GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
   GA1 S.G.T.E. **
      GA1 Ga
      GALLIUM
      Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
      20080211 BC Tref 200 -> 298.15
   IN1P1 I. BARIN 3rd. Edition
      IN1P1 INP InP
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
   IN1 S.G.T.E. **
      IN1 In
      INDIUM
      Data from SGTE Unary DB
 -OK-
Pressure /100000/: 100000
Low temperature limit /298.15/: 1000
High temperature limit /2000/: 2000
Step in temperature /100/: 100

Output file /tcex12b/:
Grapical output? /Y/: N

              O U T P U T  F R O M  T H E R M O - C A L C
              2020. 5.11                          14.48.10


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

 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
 1000.00   1.57503E+01  -4.65760E+05  -1.78780E+02  -2.86980E+05   1.86368E+02
 1100.00   1.60263E+01  -4.64172E+05  -1.77266E+02  -2.69179E+05   1.85608E+02
 1200.00   1.63030E+01  -4.62555E+05  -1.75860E+02  -2.51523E+05   1.84854E+02
 1300.00   1.65828E+01  -4.60911E+05  -1.74544E+02  -2.34004E+05   1.84111E+02
 1400.00   1.68674E+01  -4.59238E+05  -1.73305E+02  -2.16612E+05   1.83383E+02
 1500.00   1.71578E+01  -4.57537E+05  -1.72131E+02  -1.99341E+05   1.82672E+02
 1600.00   1.74548E+01  -4.55807E+05  -1.71014E+02  -1.82184E+05   1.81978E+02
 1700.00   1.77582E+01  -4.54046E+05  -1.69947E+02  -1.65136E+05   1.81301E+02
 Temperature range exceeded for GA1P1
TAB:Hit RETURN to continue
TAB: @@ ==================================================================
TAB: @@ You can list substances in the database
TAB: li-sub
   ... the command in full is LIST_SUBSTANCES
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES .....
   ... the command in full is DEFINE_SPECIES
 AG  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   AG1<G> THERMODATA
      AG1<G> Ag<G>
      SILVER <GAS>
      Modified Thermodata new assessment
   AG1 HULTGREN SELECTED VAL. SGTE **
      AG1 Ag
      SILVER
      CODATA KEY VALUE.MPT=1234.93K.
      --U.D. 30/10/85 .
      Cp from 0 to 298.5 : Hultgren 1973, Li 2007
 -OK-
With elements /*/: IN P
Exclusivly with those elements? /Y/:
```

```
IN                      P                       IN1P1
IN2                     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                      AL1CL6FE1               AL2FE1O4
AS1FE1O4                AS2FE3O8                B1FE1
B1FE2                   BA1FE1ND1O4             BA1FE2ND2O7
BR1FE1                  BR2FE1                  BR3FE1
BR4FE2                  BR6FE2                  C1FE1O3
C1FE3                   C5FE1O5                 CA1FE1O6SI2
CA1FE2O4                CA2FE2O5                CD1FE2O4
CL1FE1                  CL1FE1O1                CL2FE1
CL3FE1                  CL4FE2                  CL6FE2
CO1FE2O4                CR2FE1O4                CU1FE1O2
CU1FE1S2                CU1FE2O4                CU2FE2O4
CU5FE1S4                F1FE1                   F2FE1
F3FE1                   F4FE2                   F6FE2
FE0.875S1               FE0.947O1               FE1.04SE1
FE1/+1                  FE1/-1                  FE1H1
FE1H1O1                 FE1H1O2                 FE1H2O2
FE1H3O3                 FE1H4O6P1               FE1I1
FE1I2                   FE1I3                   FE1K1O2
FE1K2O2                 FE1K4O3                 FE1LI1O2
FE1LI5O4                FE1MO1O4                FE1NA1O2
FE1O1                   FE1O2                   FE1O3SI1
FE1O3TI1                FE1O4P1                 FE1O4S1
FE1O4V2                 FE1O4W1                 FE1O6V2
FE1P1                   FE1P2                   FE1S1
FE1S2                   FE1SE0.96               FE1SE1
FE1SE2                  FE1SI1                  FE1SI2.33
FE1SI2                  FE1TE0.9                FE1TE1
FE1TE2                  FE1TI1                  FE2
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 also tabulate data for a substance or phase. This is equivalent
TAB: @@ to those you can find in NIST-JANAF thermochemical tables for example
TAB: t-sub IN1P1
   ... the command in full is TABULATE_SUBSTANCE
   ... the command in full is REJECT
 VA  DEFINED
 REINITIATING GES .....
   ... the command in full is DEFINE_SPECIES
 IN1P1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

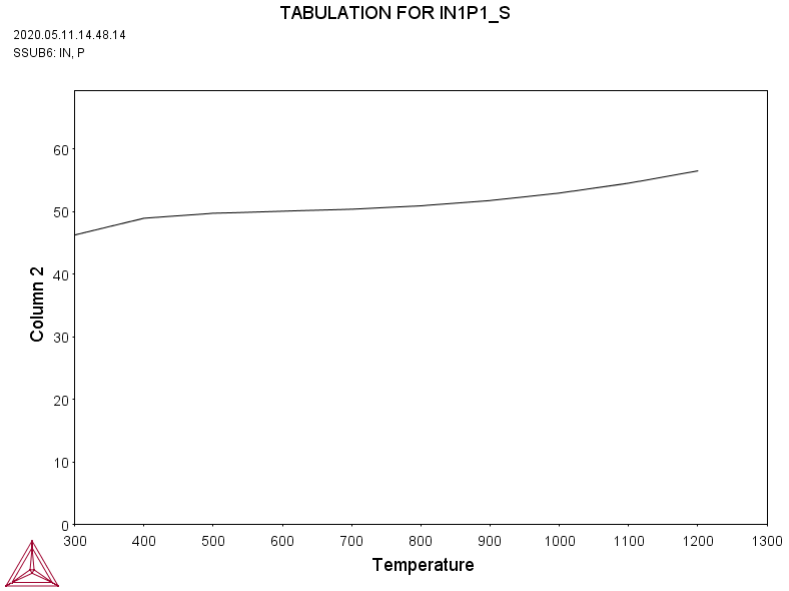
   IN1P1<G> CHATILLON(1994 March)
      IN1P1<G>
      ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
      from T.C.R.A.S.
   IN1P1 I. BARIN 3rd. Edition
      IN1P1 INP InP
      INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
      (1994)
 -OK-
Pressure /100000/: 100000
Low temperature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

               O U T P U T  F R O M  T H E R M O - C A L C
               2020. 5.11                          14.48.11

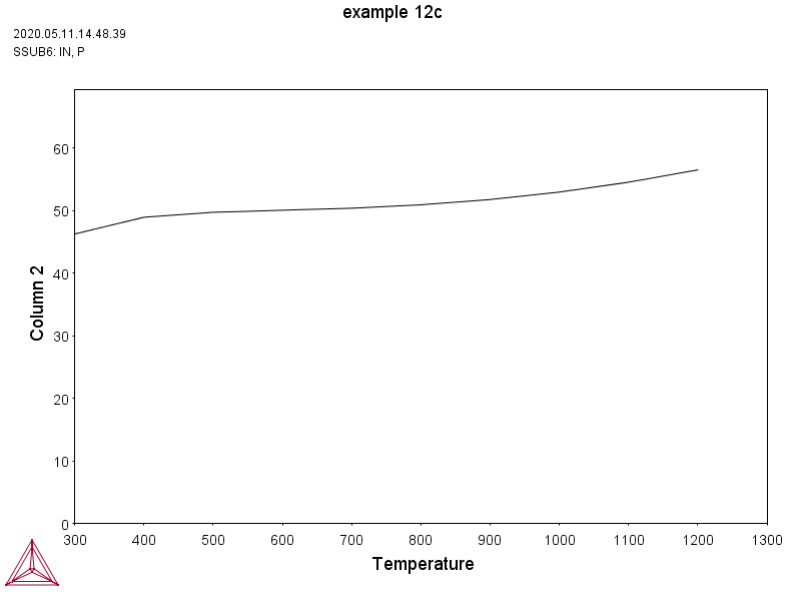

 Column 6: fef       (G-H298 )/T

 Phase : IN1P1_S                    Pressure :      100000.00
 Specie: IN1P1

 ******************************************************************************
    T      Cp            H             S             G            fef
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  300.00   4.62734E+01  -7.44015E+04   6.42060E+01  -9.36633E+04  -6.39209E+01
  400.00   4.89412E+01  -6.96137E+04   7.79614E+01  -1.00798E+05  -6.57782E+01
  500.00   4.97376E+01  -6.46723E+04   8.89845E+01  -1.09165E+05  -6.93552E+01
  600.00   5.00615E+01  -5.96811E+04   9.80837E+01  -1.18531E+05  -7.34072E+01
  700.00   5.03923E+01  -5.46595E+04   1.05824E+02  -1.28736E+05  -7.74989E+01
  800.00   5.09302E+01  -4.95956E+04   1.12585E+02  -1.39664E+05  -8.14708E+01
  900.00   5.17709E+01  -4.44633E+04   1.18629E+02  -1.51229E+05  -8.52694E+01
 1000.00   5.29647E+01  -3.92297E+04   1.24142E+02  -1.63372E+05  -8.88848E+01
 1100.00   5.45403E+01  -3.38577E+04   1.29261E+02  -1.76045E+05  -9.23252E+01
 1200.00   5.65148E+01  -2.83083E+04   1.34088E+02  -1.89214E+05  -9.56061E+01
 Temperature range exceeded
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is PLOT_DIAGRAM
```




```
POST:Hit RETURN to continue
POST:
POST: set-title example 12c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 *** ERROR  3004 IN LPOSTP:  NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: back

TAB: @@ ====================================================================
TAB: @@ In order to obtain the partial pressure of a species in
TAB: @@ the gas in its pure condensed 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 GES .....
   ... the command in full is DEFINE_SPECIES
 H1K1O1  DEFINED
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   H1K1O1<G> J. Phys. Chem. Ref. Data
      H1K1O1<G>
      Data taken from JPCRD, 26, 4 1031-1110 (1997)
   H1K1O1 J. Phys. Chem. Ref. Data
```

```
      H1K1O1
      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

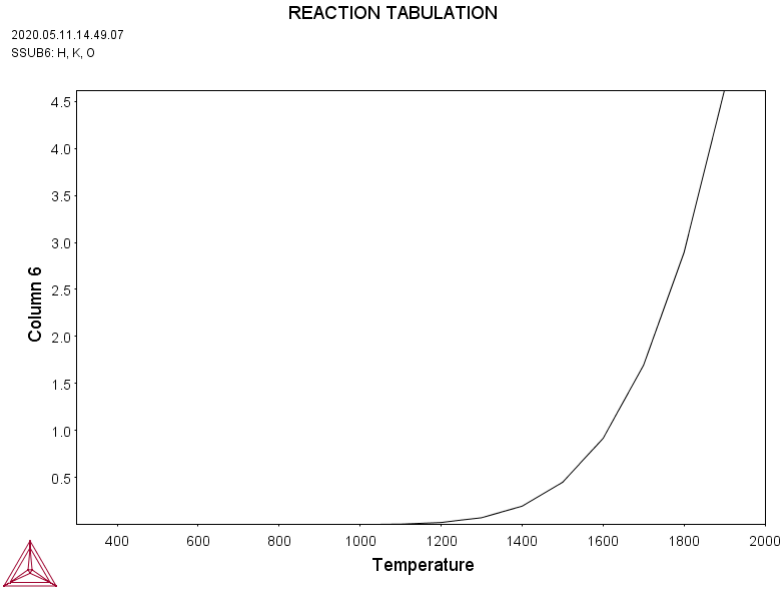
Output file /tcex12c/: tcex12d
Grapical output? /Y/: Y
Plot column? /2/: 6

               O U T P U T   F R O M   T H E R M O - C A L C
               2020. 5.11                          14.49. 2

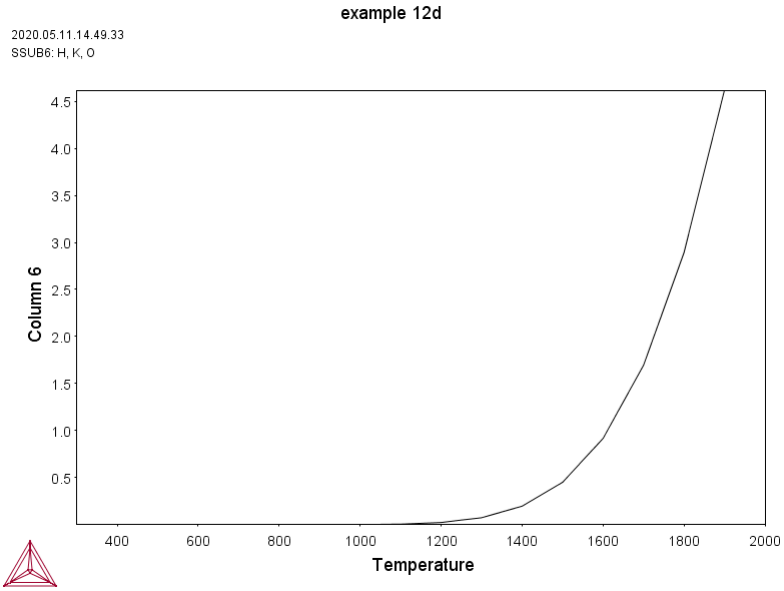

 Column 6: pp        EXP(-G/R/T )
 Reaction:  H1K1O1=H1K1O1<G>
 H1K1O1 stable as H1K1O1_S
 H1K1O1<GAS>

 ******************************************************************************
    T      Delta-Cp      Delta-H       Delta-S       Delta-G       pp
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ******************************************************************************
  300.00  -1.97899E+01   1.92543E+05   1.56915E+02   1.45469E+05   4.70147E-26
  400.00  -2.31294E+01   1.90409E+05   1.50797E+02   1.30090E+05   1.02900E-17
  500.00  -2.73216E+01   1.87890E+05   1.45195E+02   1.15293E+05   9.03075E-13
  517.   ---- H1K1O1 becomes H1K1O1_S2 ,delta-H =   5600.00
  600.00  -2.71797E+01   1.79542E+05   1.29351E+02   1.01932E+05   1.33747E-09
  680.   ---- H1K1O1 becomes H1K1O1_L ,delta-H =   7900.00
  700.00  -3.36564E+01   1.68804E+05   1.13354E+02   8.94566E+04   2.11269E-07
  800.00  -3.31914E+01   1.65462E+05   1.08890E+02   7.83499E+04   7.66317E-06
  900.00  -3.27453E+01   1.62165E+05   1.05007E+02   6.76592E+04   1.18375E-04
 1000.00  -3.22973E+01   1.58913E+05   1.01580E+02   5.73333E+04   1.01226E-03
 1100.00  -3.18358E+01   1.55706E+05   9.85231E+01   4.73310E+04   5.65583E-03
 1200.00  -3.13536E+01   1.52547E+05   9.57735E+01   3.76185E+04   2.30437E-02
 1300.00  -3.08482E+01   1.49436E+05   9.32837E+01   2.81676E+04   7.38312E-02
 1400.00  -3.03294E+01   1.46378E+05   9.10171E+01   1.89543E+04   1.96257E-01
 1500.00  -2.98854E+01   1.43368E+05   8.89402E+01   9.95788E+03   4.50033E-01
 1600.00  -2.94990E+01   1.40399E+05   8.70240E+01   1.16091E+03   9.16434E-01
 1700.00  -2.91580E+01   1.37467E+05   8.52461E+01  -7.45152E+03   1.69415E+00
 1800.00  -2.88535E+01   1.34567E+05   8.35882E+01  -1.58923E+04   2.89182E+00
 1900.00  -2.85787E+01   1.31695E+05   8.20357E+01  -2.41727E+04   4.61888E+00
 Temperature range exceeded for H1K1O1

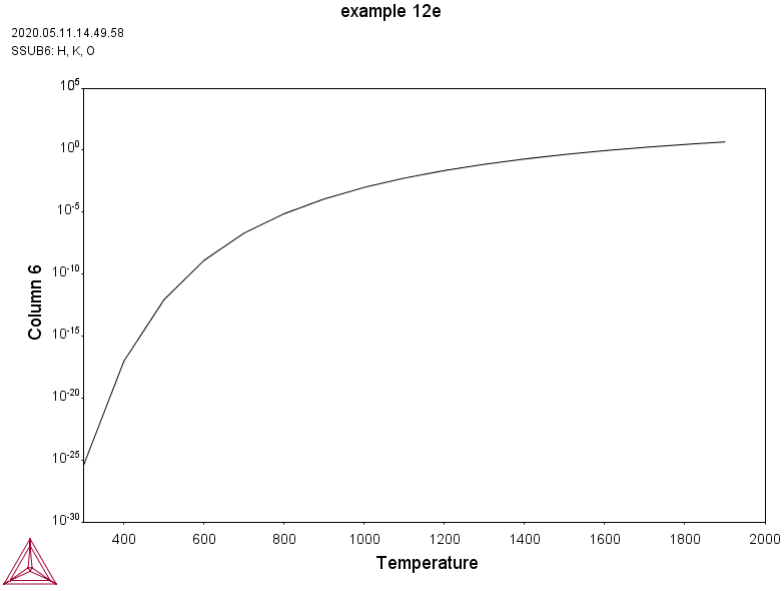
   ... the command in full is QUICK_EXPERIMENTAL_PLOT
   ... the command in full is SET_SCALING_STATUS
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-title example 12d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 *** ERROR  3004 IN LPOSTP:  NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 12e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 *** ERROR  3004 IN LPOSTP:  NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex13

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex13\tcex13.TCM"
SYS: set-echo
SYS:
SYS: @@ Calculating the binary Al-Ti phase diagram and its G curve
SYS:
SYS: @@ This example calculates an Al-Ti binary phase diagram and
SYS: @@ G curve using the BINARY module.
SYS:
SYS: set-log ex13,,,
SYS: GO BIN
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC  Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: ?
 The following assessed systems
  AG-AL AG-AU AG-BI AG-CU AG-GE AG-IN AG-IR AG-MG AG-OS AG-PB AG-PD AG-PT
  AG-RH AG-RU AG-SB AG-SI AG-SN AG-TI AG-TL AG-ZN AG-ZR AL-AS AL-AU  AL-B
  AL-BI  AL-C AL-CA AL-CE AL-CO AL-CR AL-CU AL-FE AL-GA AL-GE AL-IN AL-LI
  AL-MG AL-MN AL-MO  AL-N AL-NB AL-ND AL-NI  AL-O  AL-P AL-PB AL-SB AL-SI
  AL-SN AL-TA AL-TI  AL-V  AL-W  AL-Y AL-ZN AL-ZR AS-AU AS-CU AS-FE AS-GA
  AS-GE AS-IN  AS-P AS-SB AU-BI  AU-C AU-CR AU-CU AU-GE AU-IN AU-PB AU-PD
  AU-RH AU-RU AU-SB AU-SI AU-TE AU-TL   B-C  B-CO  B-CR  B-FE  B-HF  B-MG
  B-MO   B-N  B-ND  B-NI  B-SC  B-SI  B-TI   B-V   B-W BA-CU BA-EU BA-SR
  BA-Y BI-CU BI-GA BI-GE BI-HG BI-IN  BI-K BI-MG  BI-O BI-PB BI-SB BI-SI
  BI-SN BI-TL BI-ZN  C-CO  C-CR  C-CU  C-FE  C-HF  C-MN  C-MO  C-NB  C-NI
  C-PB  C-SI  C-TA  C-TI   C-V   C-W   C-Y  C-ZR CA-CU CA-MG CA-PB CA-SI
  CA-ZN CD-GA CD-GE CD-HG CD-IN CD-PB CD-SB CD-SN CD-TE CD-ZN CE-MG CO-CR
  CO-CU CO-DY CO-FE CO-IN CO-MN CO-MO  CO-N CO-NB CO-NI CO-PD CO-PT CO-SI
  CO-TA CO-TI  CO-V  CO-W CR-CU CR-FE CR-MG CR-MN CR-MO CR-N CR-NB CR-NI
  CR-P CR-PD CR-PT CR-SI CR-SN CR-TA CR-TI  CR-V  CR-W CR-ZN CR-ZR  CS-K
  CS-NA CS-RB CU-FE CU-GE CU-IN CU-LI CU-MG CU-MN CU-N CU-NB CU-NI  CU-O
  CU-P CU-PB  CU-S CU-SB CU-SI CU-SN CU-SR CU-TI CU-TL  CU-V  CU-Y CU-ZN
  CU-ZR DY-ER DY-HO ER-HO ER-TB FE-MG FE-MN FE-MO  FE-N FE-NB FE-ND FE-NI
  FE-O  FE-P FE-PB FE-PD FE-PR FE-PT  FE-S FE-SI FE-SN FE-TI  FE-V  FE-W
  FE-ZN FE-ZR GA-GE GA-HG GA-IN GA-P GA-PB GA-SB GA-SN GA-TE GA-ZN GE-IN
  GE-PB GE-SB GE-SI GE-SN GE-TE GE-TL GE-ZN  H-NB  H-ZR HF-TA HF-SI HF-TI
  HG-PB HO-TB  IN-P IN-PB IN-SB IN-SI IN-SN IN-ZN IR-PD  K-RB LA-NI LI-MG
  LI-ZR MG-MN MG-NI  MG-O MG-SC MG-SI  MG-Y MG-ZN MG-ZR MN-MO  MN-N  MN-O
  MN-PB MN-SI MN-TI  MN-V  MN-Y MN-ZR  MO-N MO-NB MO-NI MO-SI MO-TA MO-TI
  MO-W  N-NB  N-NI  N-TA  N-TI   N-V   N-W NA-RB NB-NI  NB-O NB-TI  NB-V
  NB-W NB-ZR ND-PR ND-SB  NI-P NI-PD NI-SI NI-TA NI-TI  NI-V  NI-W  NI-Y
  NI-ZR  O-PB  O-SN  O-SR  O-TI   O-Y  O-ZR  P-SB  P-SI PB-PD PB-SB PB-SI
  PB-SN PB-TL PB-ZN PD-RU PD-SN PR-SB PT-RH PT-RU RE-TA RE-W SB-SI SB-SN
  SB-ZN SE-SN SE-TE SE-TL SI-SN SI-TA SI-TE SI-TI  SI-U  SI-V  SI-W  SI-Y
  SI-ZN SI-ZR SN-TI SN-ZN SN-ZR TA-TI  TA-V  TA-W TA-ZR TE-ZN  TI-V  TI-W
  TI-ZR  U-ZR  V-ZR  Y-ZR

First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/:
   ... the command in full is REJECT
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES .....
   ... the command in full is DEFINE_ELEMENTS
 AL                      TI  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  CBCC_A12                CUB_A13
 B11_CUTI                B32_ALLI                C14_LAVES
 C15_LAVES               C16_AL2CU               C36_LAVES
 D019_AL1M3              D019_SNTI3              D022_AL3M1
 D1A_CU4TI               D513_AL3NI2             D88_SI3TI5
 L10_ALTI                AL11TI5                 AL2TI
 AL5FE4                  ALCE_AMORPHOUS          MTI2
   REJECTED
 LIQUID:L  RESTORED
 AL11TI5  RESTORED
 AL2TI  RESTORED
 D022_AL3M1  RESTORED
 D019_AL1M3  RESTORED
 L10_ALTI  RESTORED
 A2_BCC  RESTORED
 BCC_B2  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
   ... the command in full is GET_DATA
14:52:00,380 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
```

```
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

 'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
 'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
 'N Saunders, COST 507 (1998) ISBN 92-828-3902-8 p 89-94; Al-Ti'
 'N. Dupin, I. Ansara, Z. metallkd., Vol 90 (1999) p 76-85; Al-Ni'
 'A V Davydov et al, Metall Mater Trans 32A (2001)9 p 2175-2186; Co-Ti'
-OK-
  ... the command in full is SET_CONDITION
  ... 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

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

Organizing start points

Generating start point   1
Generating start point   2

Phase region boundary   1 at:   4.169E-01  1.704E+03
    LIQUID
 ** L10_ALTI
Calculated.                      7 equilibria

Phase region boundary   2 at:   3.454E-01  1.652E+03
    LIQUID
 ** AL11TI5
 ** L10_ALTI

Phase region boundary   3 at:   3.153E-01  1.652E+03
    LIQUID
 ** AL11TI5
Calculated.                      3 equilibria

Phase region boundary   4 at:   3.016E-01  1.646E+03
    LIQUID
 ** AL11TI5
 ** D022_AL3M1

Phase region boundary   5 at:   2.797E-01  1.646E+03
    LIQUID
 ** D022_AL3M1
Calculated.                     36 equilibria

Phase region boundary   6 at:   1.254E-01  9.380E+02
    LIQUID
 ** D022_AL3M1
 ** FCC_A1

Phase region boundary   7 at:   4.025E-03  9.380E+02
    LIQUID
 ** FCC_A1
Calculated                     12 equilibria

Phase region boundary   8 at:   1.287E-01  9.380E+02
    D022_AL3M1
 ** FCC_A1
Calculated..                     27 equilibria
Terminating at axis limit.

Phase region boundary   9 at:   2.981E-01  1.646E+03
    AL11TI5
 ** D022_AL3M1
Calculated.                     17 equilibria

Phase region boundary  10 at:   2.871E-01  1.269E+03
    AL11TI5
 ** AL2TI
 ** D022_AL3M1

Phase region boundary  11 at:   3.267E-01  1.269E+03
    AL11TI5
 ** AL2TI
Calculated.                      9 equilibria

Phase region boundary  12 at:   3.267E-01  1.454E+03
    AL11TI5
 ** AL2TI
 ** L10_ALTI

Phase region boundary  13 at:   3.539E-01  1.454E+03
    AL11TI5
 ** L10_ALTI
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   3.605E-01  1.454E+03
    AL2TI
 ** L10_ALTI
Calculated..                     48 equilibria
Terminating at axis limit.

Phase region boundary  15 at:   2.937E-01  1.269E+03
 ** AL2TI
```

```
    D022_AL3M1
 Calculated..                      40 equilibria
 Terminating at axis limit.

 Phase region boundary  16 at:   3.454E-01  1.652E+03
    LIQUID
  ** L10_ALTI
 Calculated.                       9 equilibria

 Phase region boundary  17 at:   4.476E-01  1.717E+03
    LIQUID
  ** HCP_A3
  ** L10_ALTI

 Phase region boundary  18 at:   4.672E-01  1.717E+03
    LIQUID
  ** HCP_A3
 Calculated.                       4 equilibria

 Phase region boundary  19 at:   5.157E-01  1.776E+03
    LIQUID
  ** BCC_B2
  ** HCP_A3

 Phase region boundary  20 at:   5.233E-01  1.776E+03
    LIQUID
  ** BCC_B2
 Calculated                     43 equilibria

 Phase region boundary  21 at:   5.477E-01  1.776E+03
  ** BCC_B2
    HCP_A3
 Calculated                     41 equilibria

 Phase region boundary  22 at:   4.784E-01  1.717E+03
  ** HCP_A3
    L10_ALTI
 Calculated.                      14 equilibria

 Phase region boundary  23 at:   5.545E-01  1.399E+03
  ** D019_AL1M3
  ** HCP_A3
    L10_ALTI

 Phase region boundary  24 at:   5.596E-01  1.399E+03
  ** D019_AL1M3
    L10_ALTI
 Calculated..                      45 equilibria
 Terminating at axis limit.

 Phase region boundary  25 at:   5.977E-01  1.399E+03
  ** D019_AL1M3
    HCP_A3
 Calculated..                      63 equilibria
 Terminating at axis limit.

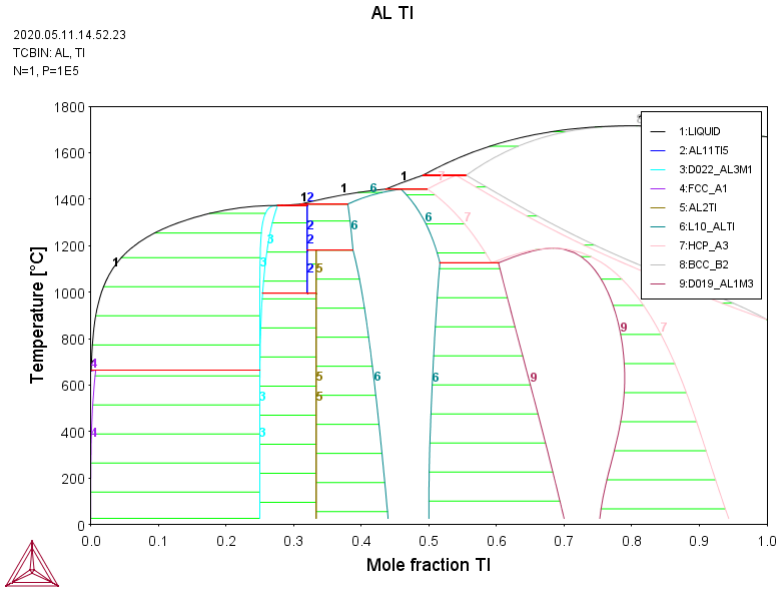
 Phase region boundary  26 at:   4.169E-01  1.704E+03
    LIQUID
  ** L10_ALTI
 Calculated.                       4 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\BINARY_002.POLY3
 CPU time for mapping                    5 seconds
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

  POSTPROCESSOR VERSION 3.2

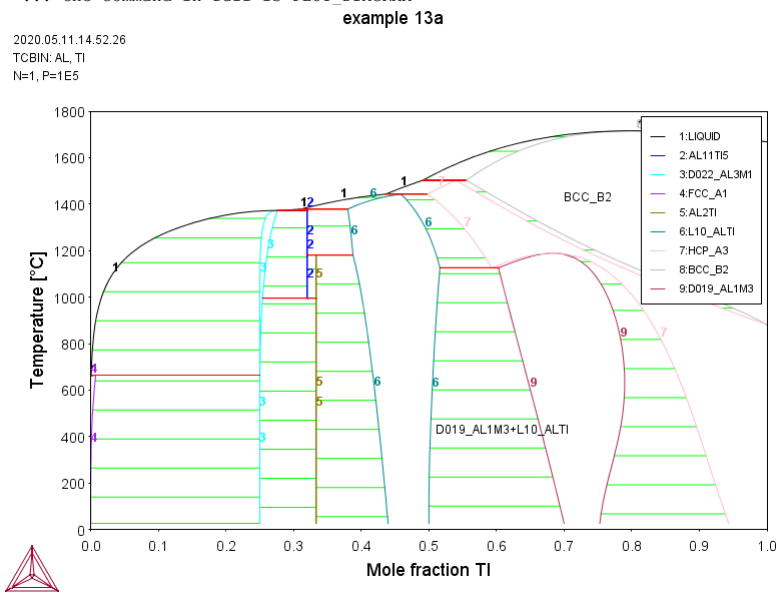
 Setting automatic diagram axes

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

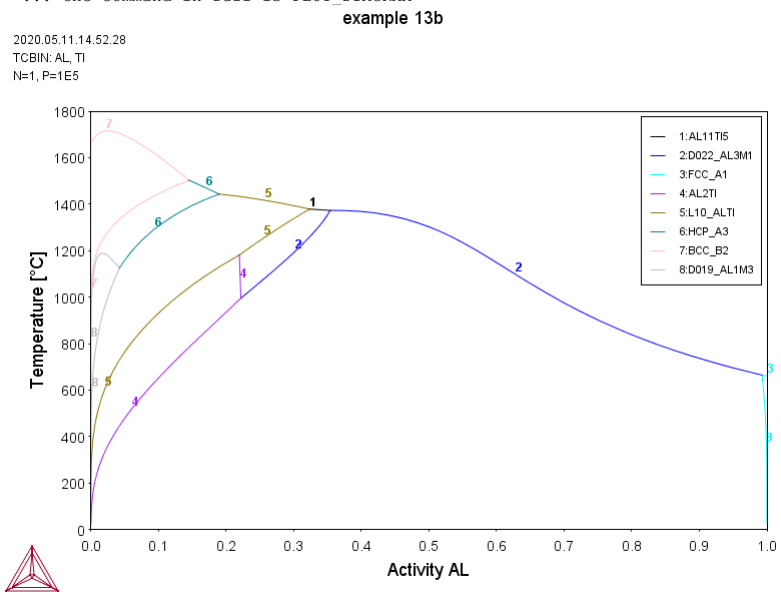



```
POST: @@ Set some phase labels
POST: ADD
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .7 1400
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated          6074 grid points in             0 s
```

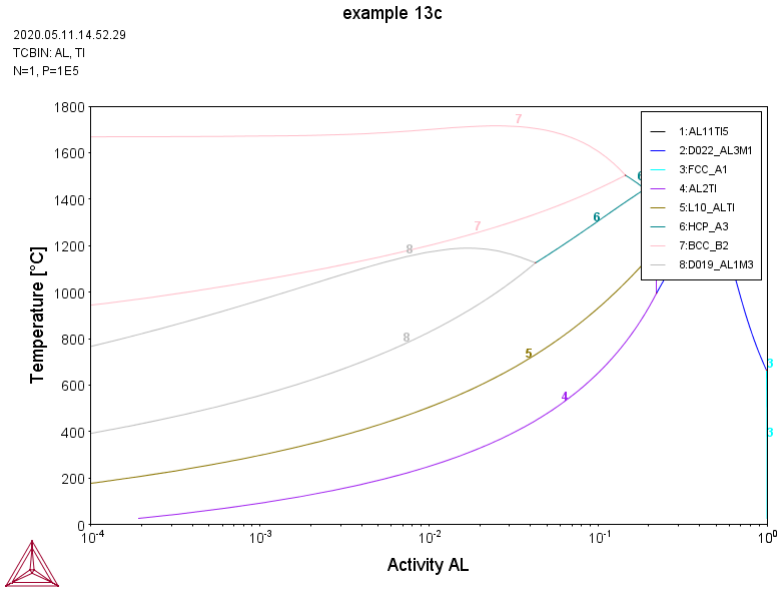
```
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_B2
Text size: /.36/:
POST: ADD
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .51 400
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
Calculated          6074 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: D019_AL1M3+L10_ALTI
Text size: /.36/:
POST: set-title example 13a
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



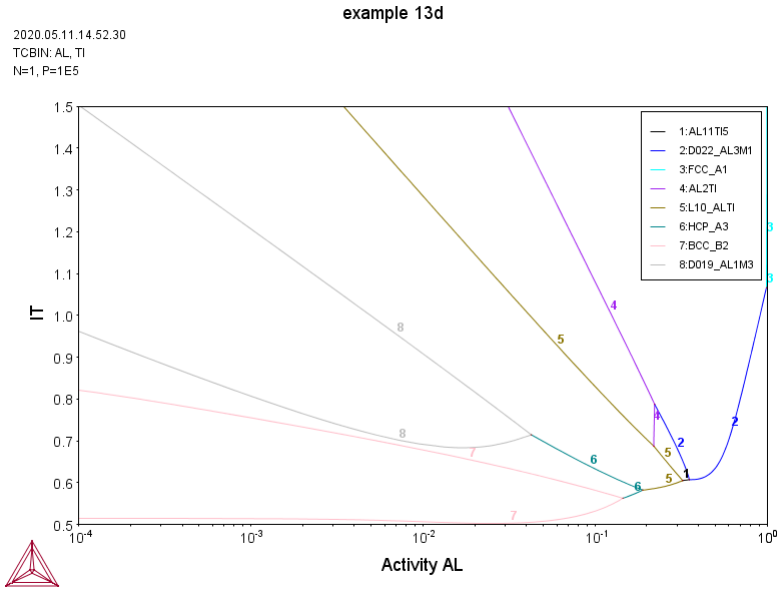

```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the activites, too
POST: S-D-A
   ... the command in full is SET_DIAGRAM_AXIS
AXIS (X, Y OR Z) : X
VARIABLE : AC
FOR COMPONENT : AL
POST: s-l e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13b
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: S-A-TY X
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: LOG
POST: S-S X N 1E-4 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 13c
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Now use inverse of T as y axis
POST: ent fun it=1000/T;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y it
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n .5 1.5
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 13d
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Now the G curves for the same system
POST: BA
   ... the command in full is BACK
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
SYS: GO BIN
   ... the command in full is GOTO_MODULE
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC  Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G
Temperature (C): /1000/: 1000
   ... the command in full is REJECT
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES .....
   ... the command in full is DEFINE_ELEMENTS
 AL                      TI  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
```

```
FCC_A1                  BCC_A2                  A2_BCC
HCP_A3                  HCP_ZN                  DIAMOND_A4
BCT_A5                  CBCC_A12                CUB_A13
B11_CUTI                B32_ALLI                C14_LAVES
C15_LAVES               C16_AL2CU               C36_LAVES
D019_AL1M3              D019_SNTI3              D022_AL3M1
D1A_CU4TI               D513_AL3NI2             D88_SI3TI5
L10_ALTI                AL11TI5                 AL2TI
AL5FE4                  ALCE_AMORPHOUS          MTI2
  REJECTED
LIQUID:L  RESTORED
AL11TI5  RESTORED
AL2TI  RESTORED
D022_AL3M1  RESTORED
D019_AL1M3  RESTORED
L10_ALTI  RESTORED
A2_BCC  RESTORED
BCC_B2  RESTORED
FCC_A1  RESTORED
HCP_A3  RESTORED
  ... the command in full is GET_DATA
ELEMENTS .....
SPECIES ......
PHASES .......
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
  ... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

 'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
 'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
 'N Saunders, COST 507 (1998) ISBN 92-828-3902-8 p 89-94; Al-Ti'
 'N. Dupin, I. Ansara, Z. metallkd., Vol 90 (1999) p 76-85; Al-Ni'
 'A V Davydov et al, Metall Mater Trans 32A (2001)9 p 2175-2186; Co-Ti'
-OK-
  ... the command in full is SET_CONDITION
  ... 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

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 SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
  ... the command in full is COMPUTE_EQUILIBRIUM
  ... the command in full is COMPUTE_EQUILIBRIUM
  ... the command in full is SAVE_WORKSPACES
  ... the command in full is STEP_WITH_OPTIONS

Phase Region from   0.502463     for:
    LIQUID
    BCC_B2
    D019_AL1M3
    FCC_A1
    HCP_A3
    L10_ALTI

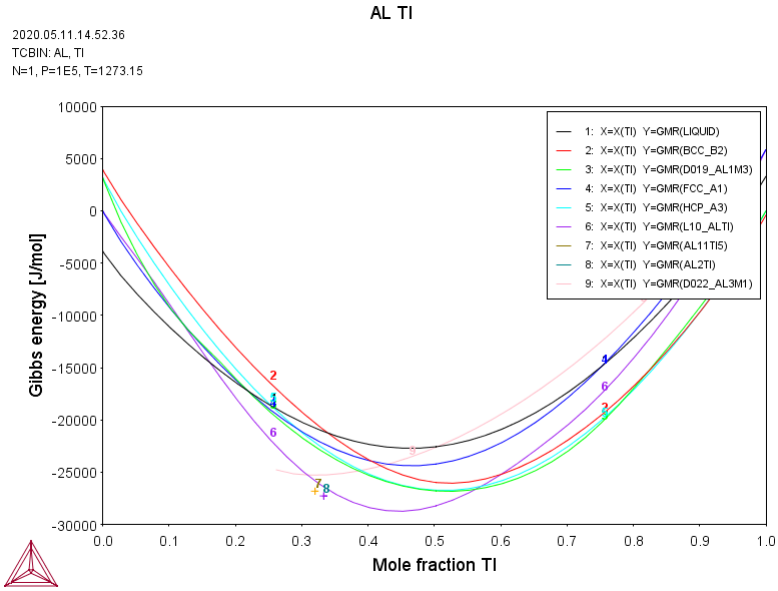
Phase Region from   0.502463     for:
    LIQUID
    BCC_B2
    D019_AL1M3
    FCC_A1
    HCP_A3
    L10_ALTI

Phase Region from   0.320000     for:
    AL11TI5

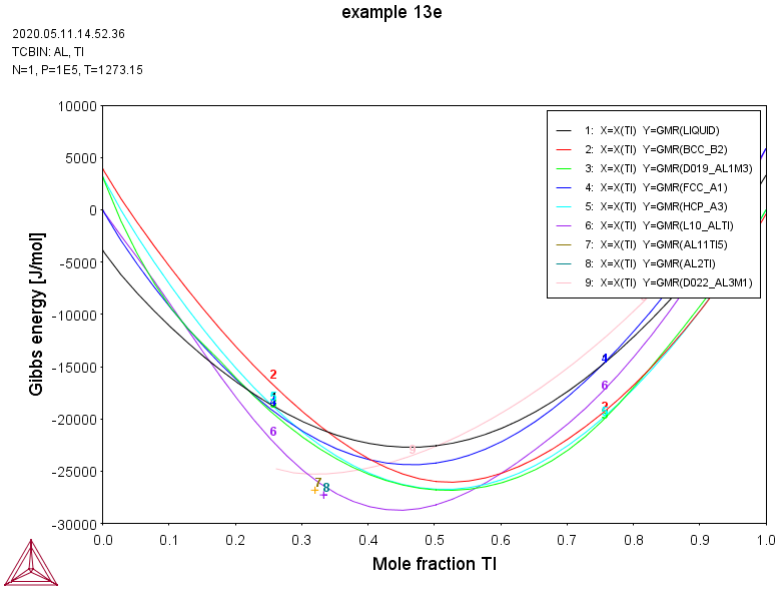
Phase Region from   0.333333     for:
    AL2TI

Phase Region from   0.636878     for:
    D022_AL3M1

Phase Region from   0.636878     for:
    D022_AL3M1
*** Buffer saved on file *** C:\Users\vagrant\AppData\Local\Temp\GCURVE_002.POLY3
 POSTPROCESSOR VERSION 3.2
  ... the command in full is SET_TIELINE_STATUS
  ... the command in full is SET_LABEL_CURVE_OPTION
  ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-label F
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 13e
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex14

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex14\tcex14.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Variations in solidification of an Al-Mg-Si alloy
SYS:
SYS: @@ This example calculates the heat and heat capacity
SYS: @@ variations during solidification of an Al-Mg-Si alloy.
SYS:
SYS: set-log ex14,,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw ALDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Aluminum Demo Database v4.0

 VA                      /-  DEFINED
TDB_ALDEMO: d-sys al cu si
   ... the command in full is DEFINE_SYSTEM
 AL                      CU                      SI
   DEFINED
TDB_ALDEMO: l-s c
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :AL CU SI:
 AL2CU_C16   :AL:AL CU SI:
 ALCU_DEL    :AL:CU:
 ALCU_EPS    :AL CU:CU:
 ALCU_ETA    :AL CU:CU:
 ALCU_ZETA   :AL:CU:
 ALZR2_B82   :AL VA:VA:
 BCC_A2      :AL CU SI VA:VA:
 BCC_B2      :AL CU SI VA:AL CU SI VA:VA:
 C14_LAVES   :AL CU:AL CU:
 C15_LAVES   :AL CU SI:AL CU SI:
 C36_LAVES   :AL CU:AL CU:
 CU15SI4_EPSILON :CU:AL SI:
 CU33SI7_DELTA :CU:SI:
 CU56SI11_GAMMA :CU SI:SI:
 CUSI_ETA    :CU:SI:
 DIAMOND_A4  :AL SI:
 FCC_A1      :AL CU SI:VA:
 GAMMA_D83   :AL SI:AL CU SI:CU:
 GAMMA_H     :AL:AL CU:CU:
 HCP_A3      :AL CU SI:VA:
TDB_ALDEMO: get
   ... the command in full is GET_DATA
14:53:57,924 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, Calphad,15 317-425 (1991)'
  'Volume data from TCFE4, 2006'
  'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
      thermal conductivity'
  'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
  'M Ghasemi, Thermo-Calc Software AB (2020)'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
  'M J Assael, J Phys Chem Ref Data 41 (2012) 033101; Cd, Co, Ga, In, Hg, Si,
       Tl, Zn'
  'I. Ansara (Editor), COST 507, (1998)'
  'M Ghasemi, Thermo-Calc Software AB (2019)'
  'C.-Y. He,Calphad, 33,200-210 (2009),Al-Cu-Si'
  'J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'
  'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),CU-Si'
  'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
      parameter, linear combination of unary volume data'
  'H-L Chen, in TCAL3.0, Assessment, extrapolation and assumption'
  'Hai-Lin Chen, electrical resistivity
       thermal conductivity (2020)'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
  'H-L Chen, Evaluation of molar volume'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
  'Nathalie Dupin, in TCNI6.0, Refinement of Al-Ni'
  'Volume data, N. Dupin 2008'
  'H-L Chen, in TCAL2.0, Assessment, extrapolation and assumption'
  'J.R.Zhao, Y.Du, to be submitted, 2010,Sn-Sr,Cu-Mg-Si'
  'W.H. Sun, unpublished (2010),Cu-Si-Zn,Cu-Ni-Zn'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'H-L Chen, in TCAL1.2, assessment of Al-Cu-Mg-Si'
 -OK-
```

```
TDB_ALDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ The composition

POLY: s-c w(si)=.09,w(cu)=.10,t=1000,p=1e5,n=1
   ... the command in full is SET_CONDITION
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 W(SI)=9E-2, W(CU)=0.1, T=1000, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         17676 grid points in             3 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     3  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: ALDEMO

 Conditions:
 W(SI)=9E-2, W(CU)=0.1, T=1000, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  2.87371E+01
 Total Gibbs energy -4.64558E+04,  Enthalpy  3.21074E+04,  Volume  1.11601E-05

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      8.6269E-01  8.1000E-01 5.0275E-03 -4.4007E+04 SER
 CU                      4.5223E-02  1.0000E-01 3.2656E-06 -1.0503E+05 SER
 SI                      9.2090E-02  9.0000E-02 7.5475E-03 -4.0629E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 2.8737E+01, Volume fraction 1.0000E+00  Mass fractions:
 AL  8.10000E-01  CU  1.00000E-01  SI  9.00000E-02
POLY:Hit RETURN to continue
POLY: @@ Set termperature as axis
POLY: 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: save tcex14 y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    1000.00
...OK

 Phase Region from    1000.00     for:
     LIQUID
 Global test at  9.20000E+02 .... OK
 Global check of adding phase at  8.41997E+02
 Calculated    18 equilibria

 Phase Region from    841.997     for:
     LIQUID
     FCC_A1
 Global check of adding phase at  8.28102E+02
 Calculated     5 equilibria

 Phase Region from    828.102     for:
     LIQUID
     DIAMOND_A4
     FCC_A1
 Global check of adding phase at  7.94799E+02
 Calculated     6 equilibria

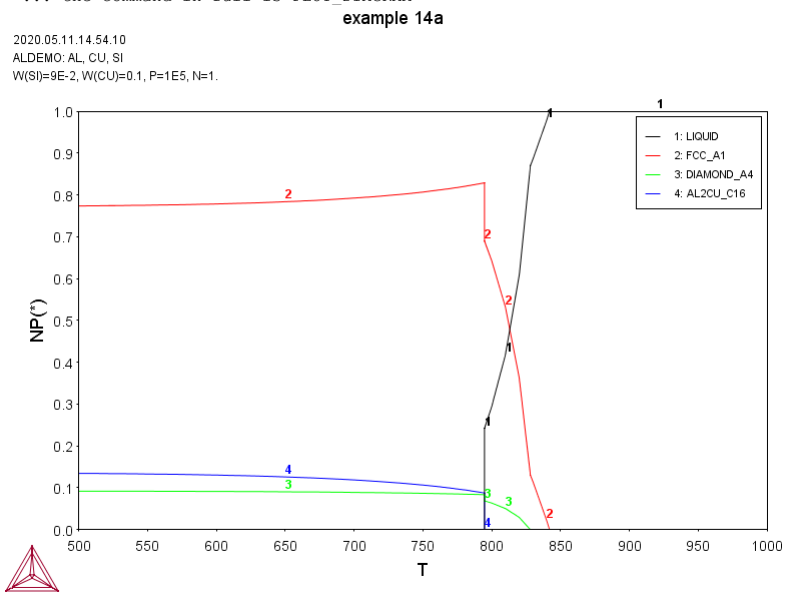
 Phase Region from    794.799     for:
     LIQUID
     AL2CU_C16
     DIAMOND_A4
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    794.799     for:
     AL2CU_C16
     DIAMOND_A4
     FCC_A1
 Global test at  7.20000E+02 .... OK
 Global test at  6.20000E+02 .... OK
 Global test at  5.20000E+02 .... OK
 Terminating at    500.000
 Calculated    33 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex14\tcex14.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

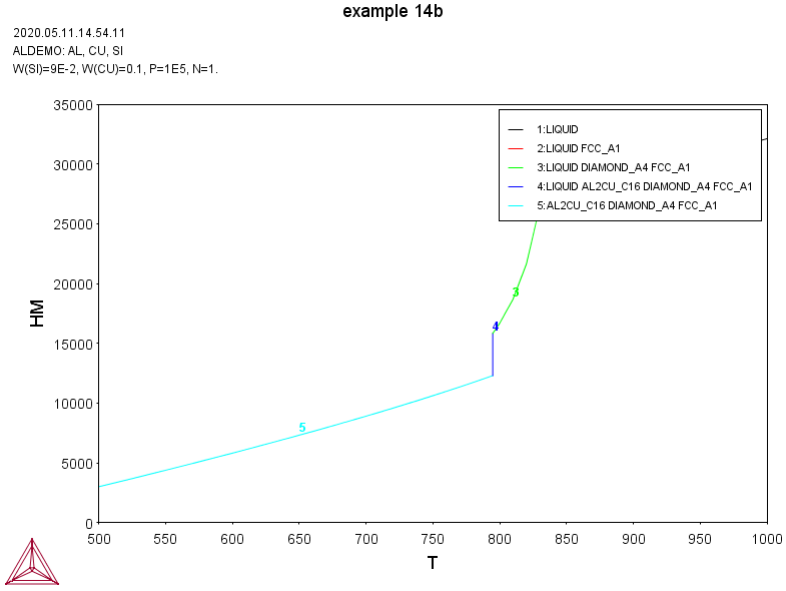
 Setting automatic diagram axes

POST: @@ Plot phase fractions
POST: S-D-A X T
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y NP(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: S-LAB D
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 14a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
```

```
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

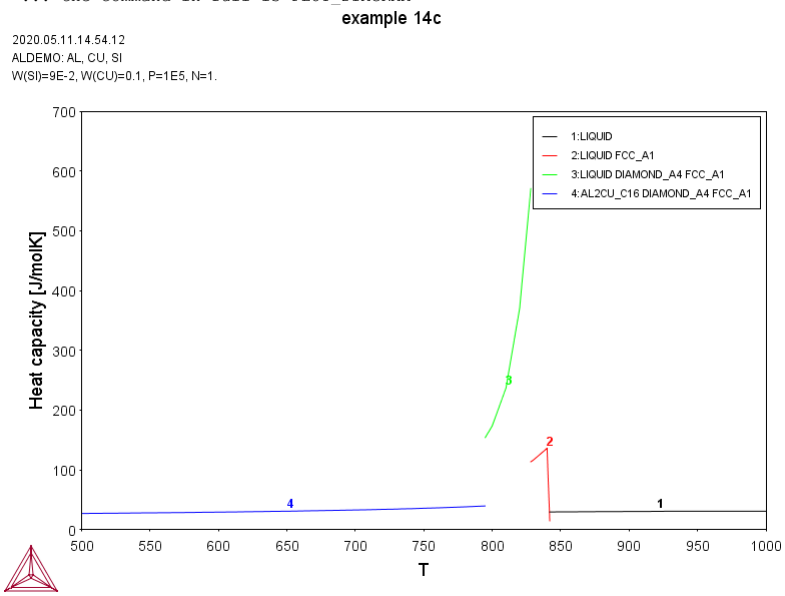



```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the total enthalpy (heat)
POST: S-D-A Y HM
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-LAB B
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 14b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the heat capacity. First this must be entered because
POST: @@ a function as derivatives cannot be plotted directly.
POST:
POST: ENT FUN CP=HM.T;
   ... the command in full is ENTER_SYMBOL
POST: S-D-A Y CP
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-S
   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC SCALING  (Y OR N) /N/: N
MIN VALUE : 0
MAX VALUE : 700
POST: S-A-T-S
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS (X, Y OR Z) : Y
AUTOMATIC AXIS TEXT  (Y OR N) /N/: N
AXIS TEXT : Heat capacity [J/molK]
POST: set-title example 14c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
```

```
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex15

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex15\tcex15.TCM.test"
SYS: SET_ECHO
SYS:
SYS: @@ Simulating the solidification of a Cr-Ni alloy with
SYS: @@ the Scheil module
SYS:
SYS: @@ This is an example of a solidification simulation
SYS: @@ of a Cr-Ni alloy. There is no back diffusion in the
SYS: @@ solid, i.e. Scheil-Gulliver model is used.
SYS:
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: GO SCHEIL
SCHEIL: TEMPERATURE-STEP
Temperature step (C) /1/: 5
SCHEIL: START-WIZARD
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: TCFE9
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
Major element or alloy: cr
Composition input in mass (weight) percent? /Y/: n
 Composition will be taken to be in mole percent
1st alloying element: ni
Mole percent /1/: 10
2nd alloying element:
Temperature (C) /2000/: 2000
 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
 REINITIATING GES .....
 CR  DEFINED
 NI  DEFINED


 This database has following phases for the defined system

 LIQUID:L                 BCC_A2                   FCC_A1
 HCP_A3                   CBCC_A12                 CUB_A13
 SIGMA                    CHI_A12                  LAVES_PHASE_C14
 CR3SI                    NBNI3                    NI3TI
 BETA1                    GAMMA                    FLUORITE_C1:I
 ZRO2_TETR:I              M2O3C:I                  CENI2
 CENI5
Reject phase(s) /NONE/: *
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  CBCC_A12                CUB_A13
 SIGMA                   CHI_A12                 LAVES_PHASE_C14
 CR3SI                   NBNI3                   NI3TI
 BETA1                   GAMMA                   FLUORITE_C1:I
 ZRO2_TETR:I             M2O3C:I                 CENI2
 CENI5  REJECTED
Restore phase(s):: liq bcc fcc
 LIQUID:L                BCC_A2                  FCC_A1
   RESTORED
Restore phase(s): /NONE/: NONE

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

    The following phases are retained in this system:

 LIQUID:L                 BCC_A2                   FCC_A1

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

OK? /Y/: y
 GAS:G  REJECTED
14:55:36,041 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
 -OK-
Should any phase have a miscibility gap check? /N/:
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/:
```

```
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=2273.15, X(NI)=0.1, P=1E5, N=1    DEGREES OF FREEDOM 0
 PHASE CHANGE AT 2058.59459939
BCC_A2#1 forms
 Testing POLY result by global minimization procedure
Calculated           627 grid points in             0 s
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

 Phase Region from    2058.68     for:
     LIQUID
 Terminating at    2058.78
 Calculated     4 equilibria

 Phase Region from    2058.68     for:
     LIQUID
 Global check of adding phase at  2.05859E+03
 Calculated     3 equilibria

 Phase Region from    2058.59     for:
     LIQUID
     BCC_A2
 Global test at  2.01868E+03 .... OK
 Global test at  1.96868E+03 .... OK
 Global test at  1.91868E+03 .... OK
 Global check of removing phase at  1.89734E+03
 Calculated    35 equilibria

 Phase Region from    1897.34     for:
     BCC_A2
 Calculated     4 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\SCHEIL_6940.POLY3
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

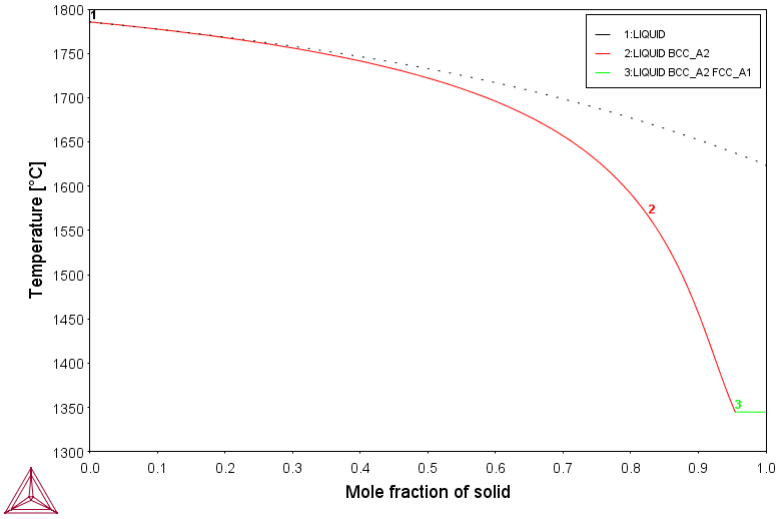
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

 An EXP file C:\Users\vagrant\AppData\Local\Temp\SCHEIL_EQ_6940.EXP
 has been created to store the equilibrium solidification results.
  CALCULATING SCHEIL SOLIDFICATION
     T(C)      fraction solid
   1785.535       0.000000
 PHASE REGION:LIQUID + BCC_A2
     T(C)      fraction solid
   1785.375      0.9239971E-03
   1780.375      0.6494391E-01
   1775.375      0.1226644
   1770.375      0.1749130
   1765.375      0.2223831
   1760.375      0.2656597
   1755.375      0.3052393
   1750.375      0.3415456
   1745.375      0.3749422
   1740.375      0.4057426
   1735.375      0.4342186
   1730.375      0.4606065
   1725.375      0.4851127
   1720.375      0.5079185
   1715.375      0.5291833
   1710.375      0.5490480
   1705.375      0.5676374
   1700.375      0.5850626
   1695.375      0.6014224
   1690.375      0.6168054
   1685.375      0.6312910
   1680.375      0.6449504
   1675.375      0.6578480
   1670.375      0.6700418
   1665.375      0.6815843
   1660.375      0.6925233
   1655.375      0.7029020
   1650.375      0.7127599
   1645.375      0.7221332
   1640.375      0.7310546
   1635.375      0.7395545
   1630.375      0.7476604
   1625.375      0.7553979
   1620.375      0.7627903
   1615.375      0.7698592
   1610.375      0.7766247
   1605.375      0.7831051
   1600.375      0.7893176
   1595.375      0.7952779
   1590.375      0.8010009
   1585.375      0.8065002
   1580.375      0.8117885
   1575.375      0.8168779
   1570.375      0.8217793
   1565.375      0.8265033
   1560.375      0.8310595
   1555.375      0.8354570
   1550.375      0.8397046
   1545.375      0.8438103
   1540.375      0.8477816
   1535.375      0.8516258
   1530.375      0.8553497
   1525.375      0.8589602
   1520.375      0.8624627
   1515.375      0.8658633
   1510.375      0.8691676
   1505.375      0.8723809
   1500.375      0.8755083
   1495.375      0.8785546
   1490.375      0.8815245
   1485.375      0.8844227
   1480.375      0.8872536
   1475.375      0.8900213
   1470.375      0.8927303
   1465.375      0.8953845
   1460.375      0.8979881
   1455.375      0.9005451
```

```
  1450.375      0.9030587
  1445.375      0.9055346
  1440.375      0.9079761
  1435.375      0.9103873
  1430.375      0.9127724
  1425.375      0.9151359
  1420.375      0.9174820
  1415.375      0.9198153
  1410.375      0.9221406
  1405.375      0.9244628
  1400.375      0.9267870
  1395.375      0.9291184
  1390.375      0.9314626
  1385.375      0.9338254
  1380.375      0.9362126
  1375.375      0.9386303
  1370.375      0.9410850
  1365.375      0.9435828
  1360.375      0.9461303
  1355.375      0.9487336
  1350.375      0.9513987
  1345.375      0.9541312
  1344.897      0.9543838
PHASE REGION:BCC_A2 + FCC_A1
    T(C)      fraction solid
  1344.738       1.000000
```

2020.05.11.14.55.52
TCFE9: CR, NI
T=2058.68, X(NI)=0.1, P=1E5, N=1




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

       The following axis variables are available

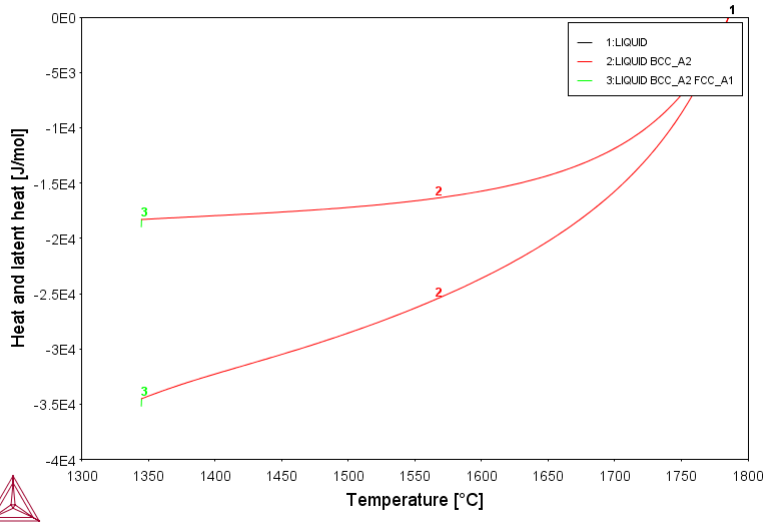
            T --- Temperature in Celsius
         NL/BL --- Mole/mass fraction of liquid
         NS/BS --- Mole/mass fraction of all solid phases
NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase
      W(ph,el) --- Weight fraction of an element in a phase
      X(ph,el) --- Mole fraction of an element in a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

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

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

POST:Hit RETURN to continue
POST: s-d-a x t
POST: s-d-a y nh
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,,,,,,,,
```

2020.05.11.14.56.30
TCFE9: CR, NI
T=2058.68, X(NI)=0.1, P=1E5, N=1




```
POST: set-inter
POST:
```

tcex16

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex16\tcex16.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Second order transition of the Al-Fe system
SYS:
SYS: @@ This example calculates the second order transition
SYS: @@ line in the Bcc field of the Al-Fe system.
SYS:
SYS: @@ Note that an SSOL database license is required to run
SYS: @@ the example.
SYS:
SYS: SET-LOG ex16,,
SYS: GO DA
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: SW SSOL6
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Alloy Solutions Database v6.0

 VA  DEFINED
 BCC_B2                  FCC_L12                 FCC_COV
 FCC_AUCU                HCP_ORD  REJECTED
 GAS:G  REJECTED
TDB_SSOL6: D-SYS AL FE
   ... the command in full is DEFINE_SYSTEM
 AL                      FE  DEFINED
TDB_SSOL6: REJ PH /ALL
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 B2_BCC                  HCP_A3                  HCP_ZN
 DHCP                    DIAMOND_A4              BCT_A5
 TETRAGONAL_U            CBCC_A12                CUB_A13
 ORTHORHOMBIC_A20        RHOMBO_C19              LAVES_C14
 LAVES_C15               LAVES_C36               M4N
 ALM_D019                ALCE_AMORPHOUS          ALCR2
 AL4CR                   AL8CR5_BETA             AL8CR5_ALPHA
 AL11CR2                 AL7CR                   ALCU_THETA
 AL2FE                   AL5FE2                  AL5FE4
 AL13FE4                 ALLI                    AL4MN
 AL6MN                   AL11MN4                 AL12MN
 ALNB3                   AL3NB                   AL3NI2
 ALPT3                   ALTI                    CR3SI_A15
 D_GAMMA                 FEPD                    FEPD3
 FESB                    FEU6                    FE2U
 FEUZR_DELTA             FEZR2                   FEZR3
   REJECTED
TDB_SSOL6: @@ The BCC phase has B2 ordering in this system.
TDB_SSOL6: @@ Note that this is modelled with two sublattices with
TDB_SSOL6: @@ both components in both sublattices
TDB_SSOL6:
TDB_SSOL6: REST PH LIQ BCC_B2 BCC_A2
   ... the command in full is RESTORE
 LIQUID:L                BCC_B2                  BCC_A2
   RESTORED
TDB_SSOL6: LI-SYS
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 LIQUID:L    :AL FE:
 BCC_A2      :AL FE:VA:
 BCC_B2      :AL FE:AL FE:VA:
TDB_SSOL6: GET
   ... the command in full is GET_DATA
14:58:09,073 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 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
 Creating a new composition set BCC_B2#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Data for the Al-Fe system were from an unpublished assessment of M
      Seiersten published in the COST507 final report: COST507
      Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,
       AT Dinsdale and MH Rand, July 1998, EUR18499. >> Al-Fe '
 -OK-
TDB_SSOL6: GO P-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: li-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 BCC_B2#2                ENTERED      0.000000E+00    0.000000E+00
 BCC_B2#1                ENTERED      0.000000E+00    0.000000E+00
```

```
 LIQUID                   ENTERED      0.000000E+00    0.000000E+00
POLY:

POLY: advanced global_minimization y 10000
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY:
POLY: @@ Set conditions where the BCC phase should be ordered
POLY: SET-COND P=1E5,N=1,T=400,X(AL)=.4
   ... the command in full is SET_CONDITION
POLY: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         10026 grid points in             3 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     4  s
POLY: @@ Use option N in order to see how Al and Fe distribute
POLY: @@ on the sublattices
POLY:
POLY: LIST-EQ
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: N
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL6

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

 Temperature    400.00 K (   126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.43010E+01
 Total Gibbs energy -3.81486E+04,  Enthalpy -2.55850E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      4.0000E-01  2.4362E-01 4.1973E-08 -5.6493E+04 SER
 FE                      6.0000E-01  7.5638E-01 4.1248E-04 -2.5919E+04 SER

 BCC_B2#2                 ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.4301E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  7.56376E-01  AL  2.43624E-01
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 AL  7.99996E-01  FE  2.00004E-01
 Sublattice  2,  Number of sites  5.0000E-01
 FE  9.99996E-01  AL  4.22881E-06
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Change the condition of the Al amount so that the
POLY: @@ site-fractions in the two sublattices will have a
POLY: @@ certain difference. If they are the same, the BCC
POLY: @@ phase is disordered. BCC_B2#2 is the default
POLY: @@ ordered phase.
POLY:
POLY: SET-COND X(AL)=NONE
   ... the command in full is SET_CONDITION
POLY: SET-COND Y(BCC_B2#2,FE#1)-Y(BCC_B2#2,FE#2)=-0.1
   ... the command in full is SET_CONDITION
POLY: C-S P BCC_B2#1=SUS
   ... the command in full is CHANGE_STATUS
POLY: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
    26 ITS,  CPU TIME USED   0 SECONDS
POLY: LIST-EQ
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/:Hit RETURN to continue
Options /VWNS/: @@ Set a smaller difference. This is as close to the
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL6

 Conditions:
 P=1E5, N=1, T=400, Y(BCC_B2#2,FE)-Y(BCC_B2#2,FE#2)=-0.1
 DEGREES OF FREEDOM 0

 Temperature    400.00 K (   126.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.36842E+01
 Total Gibbs energy -1.86969E+04,  Enthalpy -4.69474E+03,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      7.4926E-02  3.7658E-02 7.3790E-14 -1.0056E+05 SER
 FE                      9.2507E-01  9.6234E-01 2.6569E-02 -1.2066E+04 SER

 BCC_B2#2                 ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3684E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  9.62342E-01  AL  3.76585E-02
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  8.75074E-01  AL  1.24926E-01
 Sublattice  2,  Number of sites  5.0000E-01
 FE  9.75074E-01  AL  2.49265E-02
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY: @@ second order transition as it is possible to be
POLY:
POLY: SET-COND Y(BCC_B2#2,FE#1)-Y(BCC_B2#2,FE#2)=1E-4
   ... the command in full is SET_CONDITION
POLY: COMP-EQ
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
 Using already calculated grid
    14 ITS,  CPU TIME USED   0 SECONDS
POLY: @@ Now vary the temperature using these conditions
POLY: 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: @@ Always save before STEP or MAP (unless you want to
POLY: @@ overlay the new results on some previous results)
POLY:
```

```
POLY: SAVE tcex16 Y
   ... the command in full is SAVE_WORKSPACES
POLY: STEP NORMAL
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    400.000
...OK

 Phase Region from    400.000     for:
     BCC_B2#2
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
 Global test at  1.28000E+03 .... OK
 Global test at  1.38000E+03 .... OK
 Global test at  1.48000E+03 .... OK
 Global test at  1.58000E+03 .... OK
 Global check of adding phase at  1.64515E+03
 Calculated   127 equilibria

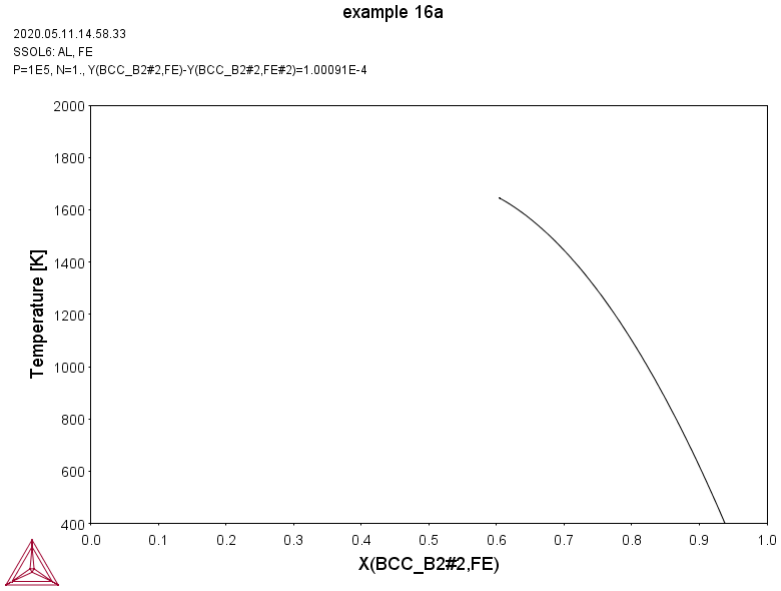
 Phase Region from    1645.15     for:
     LIQUID
     BCC_B2#2
 Global check of removing phase at  1.64515E+03
 Calculated     3 equilibria

 Phase Region from    1645.15     for:
     BCC_B2#2
 Global check of adding phase at  1.64515E+03
 Calculated     3 equilibria

 Phase Region from    1645.15     for:
     LIQUID
     BCC_B2#2
 Calculated     3 equilibria
 Sorry cannot continue     0 189 1    1.6451539E+03
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex16\tcex16.POLY3
POLY: POST
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: SET-DIA-AXIS X X(BCC_B2#2,FE)
   ... the command in full is SET_DIAGRAM_AXIS
POST: SET-DIA-AXIS Y T-K
   ... the command in full is SET_DIAGRAM_AXIS
POST: SET-SCAL X N 0 1
   ... the command in full is SET_SCALING_STATUS
POST: SET-SCAL Y N 400 2000
   ... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 16a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: PLOT
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Write on file to plot with a phase diagram
POST: MAKE TCEX16
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: Y
  No such command, use HELP
POST: BACK
POLY: GO DA
   ... the command in full is GOTO_MODULE
TDB_SSOL6: @@ Get data for all phases stable in Al-Fe
TDB_SSOL6: REJ-SYS
   ... the command in full is REJECT
 VA  DEFINED
 BCC_B2                  FCC_L12                 FCC_COV
 FCC_AUCU                HCP_ORD  REJECTED
```

```
 GAS:G  REJECTED
 REINITIATING GES .....
TDB_SSOL6: D-SYS AL FE
   ... the command in full is DEFINE_SYSTEM
 AL                      FE  DEFINED
TDB_SSOL6: L-SYS
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENT
 LIQUID:L    :AL FE:
 FCC_A1      :AL FE:VA:
 BCC_A2      :AL FE:VA:
 B2_BCC      :AL:VA:
 HCP_A3      :AL FE:VA:
 HCP_ZN      :AL FE:VA:
 DHCP        :AL:
 DIAMOND_A4  :AL:
 BCT_A5      :AL:
 TETRAGONAL_U :FE:
 CBCC_A12    :AL FE:VA:
 CUB_A13     :AL FE:VA:
 ORTHORHOMBIC_A20 :FE:
 RHOMBO_C19  :AL:
 LAVES_C14   :AL FE:AL FE:
 LAVES_C15   :AL FE:AL FE:
 LAVES_C36   :AL:AL:
 M4N         :FE:VA:
 ALM_D019    :AL:AL:
 ALCE_AMORPHOUS :AL:
 ALCR2       :AL:AL:
 AL4CR       :AL:AL:
 AL8CR5_BETA :AL:AL:
 AL8CR5_ALPHA :AL:AL:
 AL11CR2     :AL:AL:
 AL7CR       :AL:AL:
 ALCU_THETA  :AL:AL:
 AL2FE       :AL:FE:
 AL5FE2      :AL:FE:
 AL5FE4      :AL FE:
 AL13FE4     :AL:FE:AL VA:
 ALLI        :AL:VA:
 AL4MN       :AL:FE:
 AL6MN       :AL:FE:
 AL11MN4     :AL:FE:
 AL12MN      :AL:FE:
 ALNB3       :AL:AL:
 AL3NB       :AL:AL:
 AL3NI2      :AL:AL:VA:
 ALPT3       :AL:AL:
 ALTI        :AL:AL:
 CR3SI_A15   :FE:AL:VA:
 D_GAMMA     :AL:
 FEPD        :FE:FE:
 FEPD3       :FE:FE:
 FESB        :FE:FE:
 FEU6        :FE:FE:
 FE2U        :FE:FE:
 FEUZR_DELTA :FE:FE:
 FEZR2       :FE:FE:
 FEZR3       :FE:FE:
TDB_SSOL6: REJ PH /ALL
   ... the command in full is REJECT
 LIQUID:L                FCC_A1                  BCC_A2
 B2_BCC                  HCP_A3                  HCP_ZN
 DHCP                    DIAMOND_A4              BCT_A5
 TETRAGONAL_U            CBCC_A12                CUB_A13
 ORTHORHOMBIC_A20        RHOMBO_C19              LAVES_C14
 LAVES_C15               LAVES_C36               M4N
 ALM_D019                ALCE_AMORPHOUS          ALCR2
 AL4CR                   AL8CR5_BETA             AL8CR5_ALPHA
 AL11CR2                 AL7CR                   ALCU_THETA
 AL2FE                   AL5FE2                  AL5FE4
 AL13FE4                 ALLI                    AL4MN
 AL6MN                   AL11MN4                 AL12MN
 ALNB3                   AL3NB                   AL3NI2
 ALPT3                   ALTI                    CR3SI_A15
 D_GAMMA                 FEPD                    FEPD3
 FESB                    FEU6                    FE2U
 FEUZR_DELTA             FEZR2                   FEZR3
   REJECTED
TDB_SSOL6: REST PH LIQ BCC_B2 FCC_A1 BCC_A2 AL13FE4 AL2FE AL5FE2 AL5FE4
   ... the command in full is RESTORE
 LIQUID:L                BCC_B2                  FCC_A1
 BCC_A2                  AL13FE4                 AL2FE
 AL5FE2                  AL5FE4  RESTORED
TDB_SSOL6: GET
   ... the command in full is GET_DATA
 REINITIATING GES .....
 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
 Creating a new composition set BCC_B2#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'Data for the Al-Fe system were from an unpublished assessment of M
      Seiersten published in the COST507 final report: COST507
      Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,
       AT Dinsdale and MH Rand, July 1998, EUR18499. >> Al-Fe '
 -OK-
TDB_SSOL6: GO P-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ Calculate an equilibrium where BCC is ordered
POLY: S-C T=1300,P=1E5,N=1,X(AL)=.3
   ... the command in full is SET_CONDITION
POLY: C-E
   ... the command in full is COMPUTE_EQUILIBRIUM
```

```
 Using global minimization procedure
Calculated         10655 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: @@ List the equilibrium. Note that option N gives the
POLY: @@ constitution of the BCC phase and this shows that the
POLY: @@ site-fractions are different in the two sublattices,
POLY: @@ i.e. the BCC is ordered
POLY:
POLY: L-E
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/: N
 Output from POLY-3, equilibrium =     1, label A0  , database: SSOL6

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

 Temperature   1300.00 K (  1026.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.71875E+01
 Total Gibbs energy -8.63003E+04,  Enthalpy  1.26381E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      3.0000E-01  1.7154E-01 3.1606E-05 -1.1200E+05 SER
 FE                      7.0000E-01  8.2846E-01 9.4427E-04 -7.5285E+04 SER

 BCC_B2#2                 ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.7187E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  8.28459E-01  AL  1.71541E-01
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  5.22550E-01  AL  4.77450E-01
 Sublattice  2,  Number of sites  5.0000E-01
 FE  8.77450E-01  AL  1.22550E-01
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Set axis
POLY: 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: 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: 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: MAP
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Trying global minimization! 3
 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
 Trying global minimization! 3
 Generating start point  25
 Generating start point  26

 Phase region boundary   1 at:   5.820E-01  5.100E+02
  ** AL2FE
     BCC_B2#2
 Calculated..                      2 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   5.820E-01  5.000E+02
  ** AL2FE
     BCC_B2#2
```

```
Calculated.                     36 equilibria

Phase region boundary   3 at:   6.023E-01  1.368E+03
 ** AL2FE
 ** AL5FE4
    BCC_B2#2

Phase region boundary   4 at:   5.672E-01  1.368E+03
 ** AL5FE4
    BCC_B2#2
Calculated.                      7 equilibria

Phase region boundary   5 at:   5.452E-01  1.496E+03
 ** LIQUID
 ** AL5FE4
    BCC_B2#2

Phase region boundary   6 at:   5.550E-01  1.496E+03
 ** LIQUID
    BCC_B2#2
Calculated                     50 equilibria

Phase region boundary   7 at:   5.842E-01  1.496E+03
 ** LIQUID
    AL5FE4
Calculated.                      6 equilibria

Phase region boundary   8 at:   6.593E-01  1.430E+03
 ** LIQUID
 ** AL5FE2
    AL5FE4

Phase region boundary   9 at:   6.744E-01  1.430E+03
 ** AL5FE2
    AL5FE4
Calculated.                      2 equilibria

Phase region boundary  10 at:   6.740E-01  1.428E+03
 ** AL2FE
 ** AL5FE2
    AL5FE4

Phase region boundary  11 at:   6.502E-01  1.428E+03
 ** AL2FE
    AL5FE4
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   6.905E-01  1.428E+03
 ** AL2FE
    AL5FE2
Calculated..                     39 equilibria
Terminating at axis limit.

Phase region boundary  13 at:   6.993E-01  1.430E+03
    LIQUID
 ** AL5FE2
Calculated.                     12 equilibria

Phase region boundary  14 at:   7.362E-01  1.424E+03
    LIQUID
 ** AL13FE4
 ** AL5FE2

Phase region boundary  15 at:   7.556E-01  1.424E+03
    LIQUID
 ** AL13FE4
Calculated.                     24 equilibria

Phase region boundary  16 at:   8.723E-01  9.271E+02
    LIQUID
 ** AL13FE4
 ** FCC_A1

Phase region boundary  17 at:   9.955E-01  9.271E+02
    LIQUID
 ** FCC_A1
Calculated                     10 equilibria

Phase region boundary  18 at:   8.813E-01  9.271E+02
    AL13FE4
 ** FCC_A1
Calculated..                     19 equilibria
Terminating at axis limit.

Phase region boundary  19 at:   7.337E-01  1.424E+03
 ** AL13FE4
    AL5FE2
Calculated..                     38 equilibria
Terminating at axis limit.

Phase region boundary  20 at:   5.820E-01  5.100E+02
 ** AL2FE
    BCC_B2#2
Calculated.                     36 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   8.364E-03  1.237E+03
    BCC_B2#1
 ** FCC_A1
Calculated                     19 equilibria

Phase region boundary  22 at:   8.364E-03  1.237E+03
    BCC_B2#1
 ** FCC_A1
Calculated                     39 equilibria

Phase region boundary  23 at:   3.562E-01  1.702E+03
 ** LIQUID
    BCC_B2#1
Calculated                     35 equilibria

Phase region boundary  24 at:   3.562E-01  1.702E+03
 ** LIQUID
    BCC_B2#1
Calculated.                     17 equilibria
```

```
Terminating at known equilibrium

Phase region boundary  25 at:   5.820E-01  5.100E+02
 ** AL2FE
    BCC_B2#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  26 at:   5.820E-01  5.100E+02
 ** AL2FE
    BCC_B2#2
Calculated.                      36 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   8.824E-01  5.100E+02
 ** AL13FE4
    FCC_A1
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:   8.824E-01  5.100E+02
 ** AL13FE4
    FCC_A1
Calculated.                      18 equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   8.824E-01  5.100E+02
 ** AL13FE4
    FCC_A1
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  30 at:   8.824E-01  5.100E+02
 ** AL13FE4
    FCC_A1
Calculated.                      18 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   5.832E-01  1.003E+03
 ** AL2FE
    BCC_B2#2
Calculated..                      22 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  32 at:   5.832E-01  1.003E+03
 ** AL2FE
    BCC_B2#2
Calculated.                      16 equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   8.722E-01  1.003E+03
    LIQUID
 ** AL13FE4
Calculated.                       5 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.722E-01  1.003E+03
    LIQUID
 ** AL13FE4
Calculated.                      28 equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   1.805E-02  1.497E+03
 ** BCC_B2#1
    FCC_A1
Calculated                      32 equilibria

Phase region boundary  36 at:   1.805E-02  1.497E+03
 ** BCC_B2#1
    FCC_A1
Calculated                      35 equilibria

Phase region boundary  37 at:   1.032E-02  1.813E+03
    LIQUID
 ** BCC_B2#1
Calculated                      13 equilibria

Phase region boundary  38 at:   1.032E-02  1.813E+03
    LIQUID
 ** BCC_B2#1
Calculated.                      44 equilibria
Calculated                      44 equilibria

Phase region boundary  39 at:   1.032E-02  1.813E+03
    LIQUID
 ** BCC_B2#1
Calculated.                      47 equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   3.201E-01  1.728E+03
    LIQUID
 ** BCC_B2#1
Calculated                      34 equilibria

Phase region boundary  41 at:   3.201E-01  1.728E+03
    LIQUID
 ** BCC_B2#1
Calculated.                      20 equilibria
Calculated                      20 equilibria

Phase region boundary  42 at:   3.201E-01  1.728E+03
    LIQUID
 ** BCC_B2#1
Calculated                      19 equilibria

Phase region boundary  43 at:   6.421E-01  1.451E+03
    LIQUID
 ** AL5FE4
Calculated.                       7 equilibria
Calculated                       7 equilibria

Phase region boundary  44 at:   6.421E-01  1.451E+03
```

```
     LIQUID
  ** AL5FE4
 Calculated.                      6 equilibria
 Terminating at known equilibrium

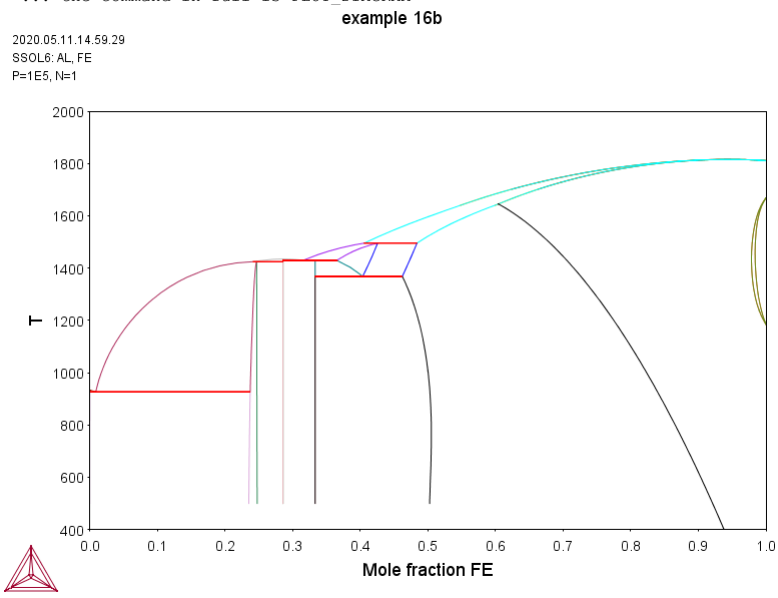
 Phase region boundary  45 at:   6.421E-01  1.451E+03
     LIQUID
  ** AL5FE4
 Calculated.                      3 equilibria
 Terminating at known equilibrium

 Phase region boundary  46 at:   8.763E-01  9.396E+02
     LIQUID
  ** AL13FE4
 Calculated.                     28 equilibria
 Terminating at known equilibrium

 Phase region boundary  47 at:   8.763E-01  9.396E+02
     LIQUID
  ** AL13FE4
 Calculated.                      2 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex16\tcex16.POLY3
 CPU time for mapping                     10 seconds
POLY:
POLY: POST
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST: S-D-A X M-F FE
   ... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y T
   ... the command in full is SET_DIAGRAM_AXIS
POST: @@ Append the previous line for the 2nd order transition
POST: A-E-D Y TCEX16
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 16b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex17

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex17\tcex17.TCM.test"
SYS: set-echo
SYS:
SYS: @@ The pseudo-binary system - CaO-SiO2
SYS:
SYS: @@ This example calculates the pseudo-binary system
SYS: @@ CaO-SiO2 using the Oxide Demo database.
SYS:
SYS: set-log ex17,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: @@ This database can be used both for pseudobinary
TDB_TCFE10: @@ systems like the one in this case, CaO-SiO2, or
TDB_TCFE10: @@ for full ternary systems like Ca-Fe-O.
TDB_TCFE10:
TDB_TCFE10: sw OXDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Oxide Demo Database v3.0

 VA                      /-  DEFINED
TDB_OXDEMO: @@ Note that /- represents the electron.
TDB_OXDEMO: d-sys ca si o
   ... the command in full is DEFINE_SYSTEM
 CA                      SI                      O
   DEFINED
TDB_OXDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
 GAS:G       :O O2:
 IONIC_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 VA SIO2:
  > Liquid metal and slag mixture.
 FCC_A1      :CA SI:O VA:
  > This is FCC_A1 solid solution.
 BCC_A2      :CA SI:O VA:
 HCP_A3      :CA SI:O VA:
 DIAMOND_FCC_A4 :SI:VA O:
  > Silicon (cF8, Fd-3m)
 QUARTZ:I    :SI+4:SIO4-4:
  > Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))
 TRIDYMITE:I :SI+4:SIO4-4:
  > Prototype SiO2 (hP12, P63/mmc)
 CRISTOBALITE:I :SI+4:SIO4-4:
  > Prototype SiO2 (cF24, Fd3m)
 CA2SIO4_ALPHA:I :CA+2:CA+2:SIO4-4:
  > This is 2CaO.SiO2. Prototype Ca2[SiO4] (hP24, P63/mmc)
 CA2SIO4_ALPHA_PRIME:I :CA+2:CA+2:SIO4-4:
  > This is 2CaO.SiO2. Prototype Sr2[SiO4] (oP52, Pnma)
 LARNITE:I   :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 (metastable at 1 atm)
 RANKINITE:I :CA+2:SI+4:O-2:
  > This is 3CaO.2SiO2 (mP48, P121/c1)
 OLIVINE:I   :CA+2:CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 and fayalite.
 PROTO_PYROXENE:I :CA+2:SI+4:O-2:
  > This is proto-enstatite with Fe solubility.
 WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (aP30, P-1)
 PSEUDO_WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (mS120, C12/c1)
 HATRURITE:I :CA+2:SIO4-4:O-2:
  > This is 3CaO.SiO2 (hR81, R3m)
 HALITE:I    :CA+2 VA:O-2:
  > This is CaO and FeO (cI2, Im-3m).
TDB_OXDEMO: @@ If we want to calculate a pseudobinary system
TDB_OXDEMO: @@ we must take away all phases and constituents that
TDB_OXDEMO: @@ make it possible for the phase to exist outside the
TDB_OXDEMO: @@ composition line from CaO to SiO2.
TDB_OXDEMO:
TDB_OXDEMO: @@ This means that for the IONIC_LIQ phase the
TDB_OXDEMO: @@ constituent Va should be suspended for systems with
TDB_OXDEMO: @@ no degree of  freedom with respect to oxygen.
TDB_OXDEMO:
TDB_OXDEMO: rej const
   ... the command in full is REJECT
PHASE: ion
SUBLATTICE NUMBER: 2
CONSTITUENT: va
 VA IN IONIC_LIQ:Y SUBLATTICE   2 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
 GAS:G       :O O2:
 IONIC_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 SIO2:
  > Liquid metal and slag mixture.
 FCC_A1      :CA SI:O VA:
  > This is FCC_A1 solid solution.
 BCC_A2      :CA SI:O VA:
 HCP_A3      :CA SI:O VA:
 DIAMOND_FCC_A4 :SI:VA O:
  > Silicon (cF8, Fd-3m)
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 QUARTZ:I    :SI+4:SIO4-4:
  > Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))
 TRIDYMITE:I :SI+4:SIO4-4:
  > Prototype SiO2 (hP12, P63/mmc)
 CRISTOBALITE:I :SI+4:SIO4-4:
  > Prototype SiO2 (cF24, Fd3m)
 CA2SIO4_ALPHA:I :CA+2:CA+2:SIO4-4:
  > This is 2CaO.SiO2. Prototype Ca2[SiO4] (hP24, P63/mmc)
 CA2SIO4_ALPHA_PRIME:I :CA+2:CA+2:SIO4-4:
  > This is 2CaO.SiO2. Prototype Sr2[SiO4] (oP52, Pnma)
 LARNITE:I   :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 (metastable at 1 atm)
 RANKINITE:I :CA+2:SI+4:O-2:
  > This is 3CaO.2SiO2 (mP48, P121/c1)
 OLIVINE:I   :CA+2:CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 and fayalite.
 PROTO_PYROXENE:I :CA+2:SI+4:O-2:
  > This is proto-enstatite with Fe solubility.
 WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (aP30, P-1)
 PSEUDO_WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (mS120, C12/c1)
 HATRURITE:I :CA+2:SIO4-4:O-2:
  > This is 3CaO.SiO2 (hR81, R3m)
 HALITE:I    :CA+2 VA:O-2:
  > This is CaO and FeO (cI2, Im-3m).
TDB_OXDEMO:Hit RETURN to continue
TDB_OXDEMO: @@ The phase names may seem unfamiliar but this is due
TDB_OXDEMO: @@ to the attempt to create a general database. Thus lime
TDB_OXDEMO: @@ (CaO) is called HALITE which is the generic phase name
TDB_OXDEMO: @@ for this structure. HALITE is also the wudstite phase
TDB_OXDEMO: @@ (FeO) and the periclase phase (MgO).
TDB_OXDEMO:
TDB_OXDEMO: @@ Note also that many phases are modelled with
TDB_OXDEMO: @@ sublattices and vacancies in order to allow for
TDB_OXDEMO: @@ non-stoichiometry in higher order systems.
TDB_OXDEMO:
TDB_OXDEMO: @@ For simplicity reject all phases except those we know
TDB_OXDEMO: @@ should be stable in this system.
TDB_OXDEMO:
TDB_OXDEMO: rej ph /all
   ... the command in full is REJECT
 GAS:G                   IONIC_LIQ:Y             FCC_A1
 BCC_A2                  HCP_A3                  DIAMOND_FCC_A4
 QUARTZ:I                TRIDYMITE:I             CRISTOBALITE:I
 CA2SIO4_ALPHA:I         CA2SIO4_ALPHA_PRIME:I   LARNITE:I
 RANKINITE:I             OLIVINE:I               PROTO_PYROXENE:I
 WOLLASTONITE:I          PSEUDO_WOLLASTONITE:I   HATRURITE:I
 HALITE:I  REJECTED
TDB_OXDEMO: rest ph ionic_liq alpha_ca2sio4 alpha_prime cristobalite halite hatrurite
   ... the command in full is RESTORE
 *** ERROR ALPHA_CA2SIO4 INPUT IGNORED
 *** ERROR ALPHA_PRIME INPUT IGNORED
 IONIC_LIQ:Y             CRISTOBALITE:I          HALITE:I
 HATRURITE:I  RESTORED
TDB_OXDEMO: rest ph larnite olivine pseudo_wollastonite quartz rankinite
   ... the command in full is RESTORE
 LARNITE:I               OLIVINE:I               PSEUDO_WOLLASTONITE:I
 QUARTZ:I                RANKINITE:I  RESTORED
TDB_OXDEMO: rest ph tridymite wollastonite
   ... the command in full is RESTORE
 TRIDYMITE:I             WOLLASTONITE:I  RESTORED
TDB_OXDEMO: @@ To avoid complications also reject the Si+4 in the
TDB_OXDEMO: @@ first sublattice in the liquid phase. When there is
TDB_OXDEMO: @@ oxygen present all Si will form SiO2 or SiO4/-4.
TDB_OXDEMO: @@ The Si+4 ion is needed only for the liquid in systems
TDB_OXDEMO: @@ without oxygen.
TDB_OXDEMO:
TDB_OXDEMO: rej const ionic_liq
   ... the command in full is REJECT
SUBLATTICE NUMBER: 1
CONSTITUENT: si+4
 SI+4 IN IONIC_LIQ:Y SUBLATTICE   1 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
 IONIC_LIQ:Y :CA+2:O-2 SIO4-4 SIO2:
  > Liquid metal and slag mixture.
 QUARTZ:I    :SI+4:SIO4-4:
  > Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))
 TRIDYMITE:I :SI+4:SIO4-4:
  > Prototype SiO2 (hP12, P63/mmc)
 CRISTOBALITE:I :SI+4:SIO4-4:
  > Prototype SiO2 (cF24, Fd3m)
 LARNITE:I   :CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 (metastable at 1 atm)
 RANKINITE:I :CA+2:SI+4:O-2:
  > This is 3CaO.2SiO2 (mP48, P121/c1)
 OLIVINE:I   :CA+2:CA+2:SI+4:O-2:
  > This is 2CaO.SiO2 and fayalite.
 WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (aP30, P-1)
 PSEUDO_WOLLASTONITE:I :CA+2:SI+4:O-2:
  > This is CaO.SiO2 (mS120, C12/c1)
 HATRURITE:I :CA+2:SIO4-4:O-2:
  > This is 3CaO.SiO2 (hR81, R3m)
 HALITE:I    :CA+2 VA:O-2:
  > This is CaO and FeO (cI2, Im-3m).
TDB_OXDEMO:Hit RETURN to continue
TDB_OXDEMO:
TDB_OXDEMO: get
   ... the command in full is GET_DATA
15:00:47,356 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set IONIC_LIQ#2
 VA IN HALITE:I SUBLATTICE   1 REJECTED
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....
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 List of references for assessed data

  'A. Dinsdale, Private Communication; liquid and solid Al2O3, CaO, MgO'
  'T.I. Barry, NPL, Unpublished work (1987); liquid and solid SiO2'
  'M. Hillert, B. Sundman and X. Wang, Calphad 15 (1991) 53-58; CaO-SiO2'
  'W. Huang, M. Hillert and X. Wang, Metall. Mater. Trans. A 26 (1995) 2293
      -2231; CaO-MgO-SiO2'
  'M. Hillert, B. Sundman and X. Wang, Metall. Trans. B 21 (1990) 303-312;
      CaO-SiO2'
  'R. Zhang, Molar volumes for oxide liquid in TCOX, Thermo-Calc Software AB,
       Sweden, 2018-2020'
  'H. Mao, B. Sundman, Z. Wang and S.K. Saxena, J. Alloys Compd., 327, 2001,
      253-262; molar volumes SiO2'
  'R. Zhang, Viscosity of liquid oxides, Thermo-Calc Software AB, 2018-2020'
 -OK-
TDB_OXDEMO: @@ There is a miscibility gap in the ionic liquid close to SiO2.
TDB_OXDEMO: @@ In this database two composition sets are created
TDB_OXDEMO: @@ automatically and one has SiO2 as a major constituent
TDB_OXDEMO:
TDB_OXDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:

POLY: @@ Define more convenient components than the elements
POLY:
POLY: list-stat cps
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)            P(Pa)
 VA                       ENTERED   SER
 CA                       ENTERED   SER
 O                        ENTERED   SER
 SI                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 WOLLASTONITE             ENTERED      0.000000E+00    0.000000E+00
 TRIDYMITE                ENTERED      0.000000E+00    0.000000E+00
 RANKINITE                ENTERED      0.000000E+00    0.000000E+00
 QUARTZ                   ENTERED      0.000000E+00    0.000000E+00
 PSEUDO_WOLLASTONITE      ENTERED      0.000000E+00    0.000000E+00
 OLIVINE                  ENTERED      0.000000E+00    0.000000E+00
 LARNITE                  ENTERED      0.000000E+00    0.000000E+00
 HATRURITE                ENTERED      0.000000E+00    0.000000E+00
 HALITE                   ENTERED      0.000000E+00    0.000000E+00
 CRISTOBALITE             ENTERED      0.000000E+00    0.000000E+00
 IONIC_LIQ#2              ENTERED      0.000000E+00    0.000000E+00
 IONIC_LIQ#1              ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CA      ENTERED    O       ENTERED    O2SI2   ENTERED    SI3     ENTERED
 CA+2    ENTERED    O-2     ENTERED    O3      ENTERED    SIO2    ENTERED
 CA1O1   ENTERED    O1SI1   ENTERED    SI      ENTERED    SIO4-4  ENTERED
 CA2     ENTERED    O2      ENTERED    SI+4    ENTERED    VA      ENTERED
 CAO     ENTERED    O2-2    ENTERED    SI2     ENTERED    VA-2    ENTERED
 E-      ENTERED    O2SI1   ENTERED    SI2O7-6 ENTERED
POLY: def-com cao sio2 o
   ... the command in full is DEFINE_COMPONENTS
POLY: l-st cps
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)            P(Pa)
 VA                       ENTERED   SER
 CAO                      ENTERED   SER
 SIO2                     ENTERED   SER
 O                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 WOLLASTONITE             ENTERED      0.000000E+00    0.000000E+00
 TRIDYMITE                ENTERED      0.000000E+00    0.000000E+00
 RANKINITE                ENTERED      0.000000E+00    0.000000E+00
 QUARTZ                   ENTERED      0.000000E+00    0.000000E+00
 PSEUDO_WOLLASTONITE      ENTERED      0.000000E+00    0.000000E+00
 OLIVINE                  ENTERED      0.000000E+00    0.000000E+00
 LARNITE                  ENTERED      0.000000E+00    0.000000E+00
 HATRURITE                ENTERED      0.000000E+00    0.000000E+00
 HALITE                   ENTERED      0.000000E+00    0.000000E+00
 CRISTOBALITE             ENTERED      0.000000E+00    0.000000E+00
 IONIC_LIQ#2              ENTERED      0.000000E+00    0.000000E+00
 IONIC_LIQ#1              ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CA      ENTERED    O       ENTERED    O2SI2   ENTERED    SI3     ENTERED
 CA+2    ENTERED    O-2     ENTERED    O3      ENTERED    SIO2    ENTERED
 CA1O1   ENTERED    O1SI1   ENTERED    SI      ENTERED    SIO4-4  ENTERED
 CA2     ENTERED    O2      ENTERED    SI+4    ENTERED    VA      ENTERED
 CAO     ENTERED    O2-2    ENTERED    SI2     ENTERED    VA-2    ENTERED
 E-      ENTERED    O2SI1   ENTERED    SI2O7-6 ENTERED
POLY:Hit RETURN to continue
POLY: s-c t=2000,p=1e5,n=1,w(sio2)=.9
   ... the command in full is SET_CONDITION
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=2000, P=1E5, N=1, W(SIO2)=0.9
 DEGREES OF FREEDOM 1
POLY: @@ There is one degree of freedom due to the oxygen. As the
POLY: @@ oxygen content is determined by the Ca/Si ration there is no
POLY: @@ possibility to vary the oxygen content in this system
POLY: @@ independently. Thus the oxygen potential can be set to any
POLY: @@ value (larger than zero).
POLY:
POLY: s-c ac(o)=1
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          1975 grid points in             1 s
    35 ITS,  CPU TIME USED   2 SECONDS
POLY:
POLY: @@ Option N is used to include information on the
POLY: @@ constitution of the phases.
POLY: l-e screen
   ... the command in full is LIST_EQUILIBRIUM
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```
Options /VWCS/: n
 Output from POLY-3, equilibrium =     1, label A0  , database: OXDEMO

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

 Temperature   2000.00 K (  1726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.96571E+01
 Total Gibbs energy -1.10541E+06,  Enthalpy -7.53274E+05,  Volume  2.62576E-05

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CAO                     1.0638E-01  1.0000E-01 6.4224E-25 -9.2632E+05 SER
 SIO2                    8.9362E-01  9.0000E-01 3.7467E-30 -1.1267E+06 SER
 O                       0.0000E+00  3.6248E-18 1.0000E+00  0.0000E+00 SER

 IONIC_LIQ#1                 Status ENTERED     Driving force  0.0000E+00
 Moles 6.7245E-01, Mass 4.0314E+01, Volume fraction 6.9348E-01  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#2                 Status ENTERED     Driving force  0.0000E+00
 Moles 3.2755E-01, Mass 1.9343E+01, Volume fraction 3.0652E-01  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:Hit RETURN to continue
POLY: @@ The result shows the expected miscibility gap. However,
POLY: @@ in some cases the first calculation may fail. In such
POLY: @@ cases try to simplify  the calculation by suspending
POLY: @@ all phases but the important ones. Save the results.
POLY:
POLY: save tcex17 y
   ... the command in full is SAVE_WORKSPACES
POLY: @@ Set the axis
POLY: 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: 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: save tcex17 Y
   ... the command in full is SAVE_WORKSPACES
POLY: 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

 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

 Phase region boundary   1 at:   1.327E-01  1.510E+03
     HALITE
  ** HATRURITE
 Calculated..                      2 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   1.327E-01  1.500E+03
     HALITE
  ** HATRURITE
 Calculated.                     48 equilibria

 Phase region boundary   3 at:   1.327E-01  2.422E+03
  ** IONIC_LIQ#2
     HALITE
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```
 ** HATRURITE

Phase region boundary   4 at:   1.433E-01  2.422E+03
 ** IONIC_LIQ#2
    HALITE
Calculated                     53 equilibria

Phase region boundary   5 at:   2.736E-01  2.422E+03
 ** IONIC_LIQ#2
    HATRURITE
Calculated.                     15 equilibria

Phase region boundary   6 at:   3.125E-01  2.160E+03
 ** IONIC_LIQ#2
    HATRURITE
 ** LARNITE

Phase region boundary   7 at:   3.061E-01  2.160E+03
    HATRURITE
 ** LARNITE
Calculated..                     34 equilibria
Terminating at axis limit.

Phase region boundary   8 at:   3.459E-01  2.160E+03
    IONIC_LIQ#2
 ** LARNITE
Calculated.                     39 equilibria

Phase region boundary   9 at:   3.845E-01  1.749E+03
    IONIC_LIQ#2
 ** LARNITE
 ** RANKINITE

Phase region boundary  10 at:   4.184E-01  1.749E+03
    IONIC_LIQ#2
 ** RANKINITE
Calculated.                      6 equilibria

Phase region boundary  11 at:   4.309E-01  1.727E+03
    IONIC_LIQ#2
 ** PSEUDO_WOLLASTONITE
 ** RANKINITE

Phase region boundary  12 at:   4.813E-01  1.727E+03
    IONIC_LIQ#2
 ** PSEUDO_WOLLASTONITE
Calculated.                     29 equilibria

Phase region boundary  13 at:   5.740E-01  1.714E+03
    IONIC_LIQ#2
 ** PSEUDO_WOLLASTONITE
 ** TRIDYMITE

Phase region boundary  14 at:   8.175E-01  1.714E+03
    IONIC_LIQ#2
 ** TRIDYMITE
Calculated.                      3 equilibria

Phase region boundary  15 at:   8.222E-01  1.744E+03
    IONIC_LIQ#2
 ** CRISTOBALITE
 ** TRIDYMITE

Phase region boundary  16 at:   8.222E-01  1.744E+03
    IONIC_LIQ#2
 ** CRISTOBALITE
Calculated.                     12 equilibria

Phase region boundary  17 at:   8.695E-01  1.959E+03
 ** IONIC_LIQ#1
    IONIC_LIQ#2
 ** CRISTOBALITE

Phase region boundary  18 at:   8.574E-01  1.959E+03
 ** IONIC_LIQ#1
    IONIC_LIQ#2
Calculated.                     26 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   9.882E-01  1.959E+03
 ** IONIC_LIQ#1
    CRISTOBALITE
Calculated                     24 equilibria

Phase region boundary  20 at:   1.000E+00  1.744E+03
 ** CRISTOBALITE
    TRIDYMITE

Phase region boundary  21 at:   7.627E-01  1.714E+03
    PSEUDO_WOLLASTONITE
 ** TRIDYMITE
Calculated..                     12 equilibria
Terminating at axis limit.

Phase region boundary  22 at:   4.671E-01  1.727E+03
 ** PSEUDO_WOLLASTONITE
    RANKINITE
Calculated..                     13 equilibria
Terminating at axis limit.

Phase region boundary  23 at:   3.828E-01  1.749E+03
    LARNITE
 ** RANKINITE
Calculated..                     14 equilibria
Terminating at axis limit.

Phase region boundary  24 at:   1.327E-01  1.510E+03
    HALITE
 ** HATRURITE
Calculated.                     47 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   1.327E-01  1.510E+03
    HALITE
 ** HATRURITE
Calculated..                      2 equilibria
```

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

Phase region boundary  26 at:   1.327E-01  1.510E+03
    HALITE
 ** HATRURITE
Calculated.                     47 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.061E-01  1.510E+03
    HATRURITE
 ** LARNITE
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:   3.061E-01  1.510E+03
    HATRURITE
 ** LARNITE
Calculated.                     34 equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  30 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated.                     13 equilibria
Calculated                     13 equilibria

Phase region boundary  31 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated.                     12 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  33 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated.                     13 equilibria
Calculated                     13 equilibria

Phase region boundary  34 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated.                     12 equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  36 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated.                     13 equilibria
Calculated                     13 equilibria

Phase region boundary  37 at:   7.627E-01  1.510E+03
 ** PSEUDO_WOLLASTONITE
    TRIDYMITE
Calculated.                     12 equilibria
Terminating at known equilibrium

Phase region boundary  38 at:   3.026E-01  2.170E+03
    IONIC_LIQ#1
 ** HATRURITE
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   3.026E-01  2.170E+03
    IONIC_LIQ#1
 ** HATRURITE
Calculated.                     14 equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   9.885E-02  2.830E+03
    IONIC_LIQ#1
 ** HALITE
Calculated.                     22 equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   9.885E-02  2.830E+03
    IONIC_LIQ#1
 ** HALITE
Calculated                     30 equilibria

Phase region boundary  42 at:   9.885E-02  2.830E+03
    IONIC_LIQ#1
 ** HALITE
Calculated.                     22 equilibria
Terminating at known equilibrium

Phase region boundary  43 at:   9.885E-02  2.830E+03
    IONIC_LIQ#1
 ** HALITE
Calculated                     30 equilibria

Phase region boundary  44 at:   5.002E-03  3.162E+03
    IONIC_LIQ#1
 ** HALITE
```

```
 Calculated                      9 equilibria

 Phase region boundary  45 at:   5.002E-03  3.162E+03
     IONIC_LIQ#1
  ** HALITE
 Calculated.                     40 equilibria
 Terminating at known equilibrium

 Phase region boundary  46 at:   3.000E-01  2.211E+03
     IONIC_LIQ#1
  ** HATRURITE
 Calculated.                     12 equilibria
 Terminating at known equilibrium

 Phase region boundary  47 at:   3.000E-01  2.211E+03
     IONIC_LIQ#1
  ** HATRURITE
 Calculated.                      4 equilibria
 Terminating at known equilibrium

 Phase region boundary  48 at:   8.337E-01  1.812E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated.                      5 equilibria
 Terminating at known equilibrium

 Phase region boundary  49 at:   8.337E-01  1.812E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated                     10 equilibria

 Phase region boundary  50 at:   8.337E-01  1.812E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated.                      9 equilibria
 Terminating at known equilibrium

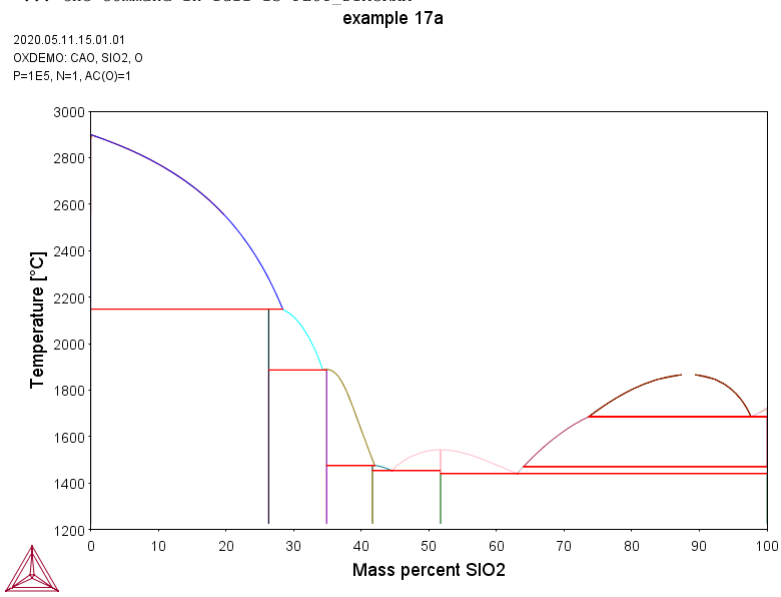
 Phase region boundary  51 at:   9.950E-01  1.978E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated                     10 equilibria

 Phase region boundary  52 at:   9.950E-01  1.978E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated.                      2 equilibria
 Terminating at known equilibrium

 Phase region boundary  53 at:   9.950E-01  1.978E+03
     IONIC_LIQ#1
  ** CRISTOBALITE
 Calculated                     24 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex17\tcex17.POLY3
 CPU time for mapping                     5 seconds
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

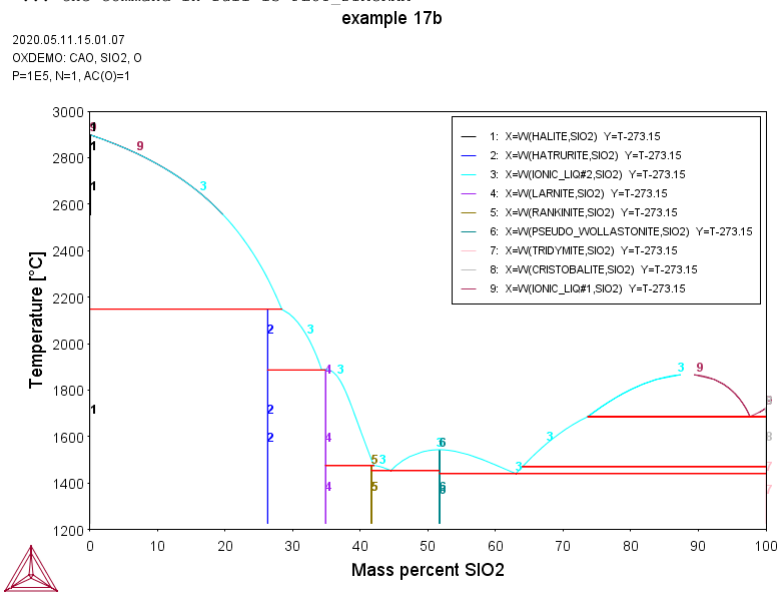
 Setting automatic diagram axes

POST: s-d-a x w-p sio2
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 17a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Indentify the phases with labels
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: f
POST:
POST: set-title example 17b
```

```
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex18

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex18\tcex18.TCM.test"
SYS: set-echo
SYS:
SYS: @@ A3 temperature of a steel
SYS:
SYS: @@ This example calculates the A3 temperature of a steel
SYS: @@ and the influence of each alloying element on
SYS: @@ this temperature
SYS:
SYS: @@ A3 temperature is the temperature where ferrite starts to
SYS: @@ form from austenite. You can easily read A3 from an Fe-C
SYS: @@ phase diagram. But for complex multicomponent steels, no
SYS: @@ simple diagram can be used.
SYS:
SYS: @@ Using POLY, it is easy to find out the influence of each
SYS: @@ alloying element on A3 temperature. This information is
SYS: @@ useful if you want to modify the compositions of a steel
SYS: @@  but keep A3 unchanged.
SYS:
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex18,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: tcfe9
 Current database: Steels/Fe-Alloys  v9.2

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


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE                M23C6                    M7C3
 M6C                      M5C2                     M3C2
 KSI_CARBIDE              Z_PHASE                  FE4N_LP1
 FECN_CHI                 SIGMA                    HIGH_SIGMA
 MU_PHASE                 CHI_A12                  LAVES_PHASE_C14
 M3SI                     MN9SI2                   MN11SI19
 MN6SI                    G_PHASE                  CR3SI
 FE2SI                    FESI2_H                  FESI2_L
 MSI                      M5SI3                    NBNI3
 NB3SI                    NB5SI3_D8L               NB5SI3_D8M
 MSI2_C40                 CRNBSI                   M11SI8
 M6SI5                    FENBSI2                  FE4NB4SI7
 FENBSI                   FE3NB4SI5                FENB2SI2
 FENB4SI                  AL4C3                    FE8SI2C
 SIC                      MN5SIC                   CRZN17
 CUZN_EPSILON             AL5FE4                   MP_B31
 M2P_C22                  FLUORITE_C1:I            ZRO2_TETR:I
 M2O3C:I                  M2O3H:I
Reject phase(s) /NONE/: ?
 FILE SYSTEM ERROR IN FILHLP
 ERROR                   1717  READING HELP FILE
Reject phase(s) /NONE/: *
 GAS:G                   LIQUID:L                 BCC_A2
 FCC_A1                  HCP_A3                   CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE               M23C6                    M7C3
 M6C                     M5C2                     M3C2
 KSI_CARBIDE             Z_PHASE                  FE4N_LP1
```

```
 FECN_CHI                SIGMA                   HIGH_SIGMA
 MU_PHASE                CHI_A12                 LAVES_PHASE_C14
 M3SI                    MN9SI2                  MN11SI19
 MN6SI                   G_PHASE                 CR3SI
 FE2SI                   FESI2_H                 FESI2_L
 MSI                     M5SI3                   NBNI3
 NB3SI                   NB5SI3_D8L              NB5SI3_D8M
 MSI2_C40                CRNBSI                  M11SI8
 M6SI5                   FENBSI2                 FE4NB4SI7
 FENBSI                  FE3NB4SI5               FENB2SI2
 FENB4SI                 AL4C3                   FE8SI2C
 SIC                     MN5SIC                  CRZN17
 CUZN_EPSILON            AL5FE4                  MP_B31
 M2P_C22                 FLUORITE_C1:I           ZRO2_TETR:I
 M2O3C:I                 M2O3H:I  REJECTED
Restore phase(s):: liq fcc_a1 bcc_a2 hcp_a3 graphite cementite m23 m7
 LIQUID:L                FCC_A1                  BCC_A2
 HCP_A3                  GRAPHITE                CEMENTITE
 M23C6                   M7C3  RESTORED
Restore phase(s): /NONE/:

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

    The following phases are retained in this system:

 LIQUID:L                 BCC_A2                   FCC_A1
 HCP_A3                   GRAPHITE                 CEMENTITE
 M23C6                    M7C3

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

OK? /Y/: Y
15:02:28,711 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set HCP_A3#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'C. Qiu, ISIJ International, 32 (1992) 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  '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'
  '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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'B.-J. Lee, Metall. Mater. Trans. A, 32A (2001) 2423-39'
  'A.V. Khvan, B. Hallstedt, CALPHAD, 40, 10-15(2013); Fe-Nb, Nb-C, Nb-N, Fe
      -Mn-Nb, Fe-Nb-C, Fe-Nb-N, Nb-C-N, Fe-Mn-Nb-C, Fe-Mn-Nb-N'
  'Thermo-Calc Software, Sweden, 2019: Volume data updated for TCFE9
      database (TCFE v9.1, June, 2019).'
  'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6
      database (TCFE v6, April, 2008).'
  'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C
      and Al-Si-C'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
  'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
  'J.G. Costa Neto, S.G. Fries, H.L. Lukas, S. Gama and G. Effenberg,
      CALPHAD, 17 (1993) 219-228; Cr-Nb'
  'B. Sundman, Private communication, (2000); Estimated Cr-Ni-Mo'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'A. V. Khvan, B. Hallstedt, CALPHAD, 39 (2012) 62-69; Fe-Nb'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
  'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
      and Fe-Mn-Nb'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'P.B. Fernandes, G. C. Coelho, F. Ferreira, C. A. Nunes, and B. Sundman,
      Intermetallics, 10 (2002) 993-999; Nb-Si'
  'Same or similar interaction as in the corresponding stable phase'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
```

```
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-Nb-V-C-N'
  'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; C-Cr-Si'
  'S. Canderyd, Report IM-2005-109, Stockholm, Sweden; Fe-Nb-C'
  'W. Huang, Z. Metallkd., 6 (1990) 397-404; Fe-Nb-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid
      C-Fe-Si description'
  'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
  'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
  'J. Miettinen, CALPHAD, 23 (2)(1999) 249-262; Cr-Fe-Si'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         10854 grid points in             3 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     3  s
POLY:

POLY: @@ In the TCFE database the number of phases is very large.
POLY: @@ It is strongly recommended that you reject all phases
POLY: @@ that you know should not be stable
POLY:
POLY: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -7.21987E+04,  Enthalpy  4.05694E+04,  Volume  7.32058E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3747E-02  3.0000E-03 1.0862E-02 -5.1634E+04 SER
 CR                      1.5877E-02  1.5000E-02 1.3241E-04 -1.0195E+05 SER
 FE                      9.5890E-01  9.7300E-01 2.0388E-03 -7.0733E+04 SER
 MN                      5.0091E-03  5.0000E-03 4.2429E-06 -1.4123E+05 SER
 NB                      5.9240E-04  1.0000E-03 1.3166E-07 -1.8088E+05 SER
 SI                      5.8788E-03  3.0000E-03 1.1006E-08 -2.0922E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.9898E-01, Mass 5.4983E+01, Volume fraction 9.9903E-01  Mass fractions:
 FE  9.73949E-01  MN  5.00487E-03  C   2.89425E-03
 CR  1.50124E-02  SI  3.00295E-03  NB  1.36838E-04

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0186E-03, Mass 5.4015E-02, Volume fraction 9.7384E-04  Mass fractions:
 NB  8.79642E-01  FE  7.30786E-03  MN  4.49817E-05
 C   1.10649E-01  CR  2.35667E-03  SI  1.99881E-09
POLY:Hit RETURN to continue
POLY: @@ Two FCC phases are stable, one with mainly Fe and
POLY: @@ one with mainly Nb and C, which is the NbC carbide.
POLY: @@ The second fcc is called FCC#2. The number after # is
POLY: @@ called composition set but can be ignored if it is unity.
POLY:
POLY: li-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 C                       ENTERED   SER
 CR                      ENTERED   SER
 FE                      ENTERED   SER
 MN                      ENTERED   SER
 NB                      ENTERED   SER
 SI                      ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 FCC_A1#2                ENTERED      0.000000E+00    1.018576E-03
 FCC_A1#1                ENTERED      0.000000E+00    9.989814E-01
 BCC_A2                  ENTERED     -1.864584E-02    0.000000E+00
 LIQUID                  ENTERED     -2.117120E-01    0.000000E+00
 HCP_A3#1                ENTERED     -3.241964E-01    0.000000E+00
 HCP_A3#2                ENTERED     -3.241964E-01    0.000000E+00
 M23C6                   ENTERED     -4.192386E-01    0.000000E+00
 CEMENTITE               ENTERED     -4.745966E-01    0.000000E+00
 M7C3                    ENTERED     -6.297003E-01    0.000000E+00
 GRAPHITE                ENTERED     -2.493419E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 C    ENTERED    C60  ENTERED    FE+2 ENTERED    MN+3 ENTERED    SI   ENTERED
 C2   ENTERED    CR   ENTERED    FE+3 ENTERED    MN+4 ENTERED    SI+4 ENTERED
 C3   ENTERED    CR+2 ENTERED    FE+4 ENTERED    NB   ENTERED    VA   ENTERED
 C4   ENTERED    CR+3 ENTERED    MN   ENTERED    NB+2 ENTERED
 C5   ENTERED    FE   ENTERED    MN+2 ENTERED    NB+4 ENTERED
POLY:
POLY: @@ Fcc appears twice in the list. The HCP phase also has
POLY: @@ two composition sets.
POLY:
POLY: @@ This result looks reasonable; save it to file
POLY: save tcex18 y
   ... the command in full is SAVE_WORKSPACES
POLY:
POLY: @@ Now calculate when bcc (ferrite) begins to form
POLY: @@ using the COMPUTE-TRANSITION command
POLY: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
 You must release one of these conditions
 T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
 P=1E5, N=1    DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
 Testing POLY result by global minimization procedure
Calculated         10854 grid points in             0 s
To form BCC_A2 the condition is set to T=1071.50342108
POLY:Hit RETURN to continue
POLY: @@ We may expect BCC to form at a lower temperature, because
```

```
POLY: @@ sometimes a higer temperature is found as there is a
POLY: @@ delta-ferrite stable at high temperatures.
POLY:
POLY: @@ Calculate the equilibrium at lower temperature again. You
POLY: @@ can do this with a SET-COND T=... command but then the
POLY: @@ temperature must be given in Kelvin. You can use the
POLY: @@ DEF-MAT command to do this in Celsius
POLY:
POLY: 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         10854 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: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -4.87884E+04,  Enthalpy  3.03124E+04,  Volume  7.17692E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3747E-02  3.0000E-03 4.4656E-02 -2.7739E+04 SER
 CR                      1.5877E-02  1.5000E-02 3.5959E-04 -7.0762E+04 SER
 FE                      9.5890E-01  9.7300E-01 4.8672E-03 -4.7516E+04 SER
 MN                      5.0091E-03  5.0000E-03 8.0911E-06 -1.0462E+05 SER
 NB                      5.9240E-04  1.0000E-03 2.9538E-09 -1.7524E+05 SER
 SI                      5.8788E-03  3.0000E-03 8.8826E-10 -1.8597E+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  9.74157E-01  MN  5.00591E-03  C   2.86358E-03
 CR  1.49681E-02  SI  3.00361E-03  NB  1.58326E-06

 FCC_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.2991E-03, Mass 6.6172E-02, Volume fraction 1.2216E-03  Mass fractions:
 NB  8.30412E-01  CR  4.14701E-02  MN  9.23349E-05
 C   1.16325E-01  FE  1.17005E-02  SI  2.55893E-10
POLY:
POLY: @@ Try a slightly different COMPUTE-TRANSITION command.
POLY: @@ This finds the first phase change in the specified
POLY: @@ direction.
POLY:
POLY: 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/: ?
 FILE SYSTEM ERROR IN FILHLP
Estimated change (with sign) /1/: -1
 PHASE CHANGE AT 1071.50341573
BCC_A2#1 forms
 Testing POLY result by global minimization procedure
Calculated         10854 grid points in             0 s
POLY: show t
   ... the command in full is SHOW_VALUE
 T=1071.5034
POLY: @@ The transition temperature to form BCC is the same.
POLY: @@ If we want it in Celsius enter a function.
POLY: enter fun tc=t-273;
   ... the command in full is ENTER_SYMBOL
POLY: show tc
   ... the command in full is SHOW_VALUE
 TC=798.50342
POLY:
POLY:Hit RETURN to continue
POLY: @@ This is the minimum temperature for hardening because
POLY: @@ below this temperature ferrite will form from austenite.
POLY: @@ Check how a small change of the composition can change
POLY: @@ this temperature. We must then set bcc as Fix and
POLY: @@ release the condition on the temperature.
POLY:
POLY: c-st p bcc_a2=fix 0
   ... the command in full is CHANGE_STATUS
POLY: s-c t=none
   ... the command in full is SET_CONDITION
POLY: @@ The change of the calculated temperature for a small
POLY: @@ change of the amount of a component can be calculated
POLY: @@ as a derivative using the dot "." between the
POLY: @@ calculated variable and the condition.
POLY:
POLY: sh t.w(mn)
   ... the command in full is SHOW_VALUE
 T.W(MN)=-2586.64
POLY: sh t.w(cr)
   ... the command in full is SHOW_VALUE
 T.W(CR)=-788.76101
POLY: sh t.w(nb)
   ... the command in full is SHOW_VALUE
 T.W(NB)=3020.6489
POLY: sh t.w(c)
   ... the command in full is SHOW_VALUE
 T.W(C)=-21904.118
POLY: sh t.w(si)
   ... the command in full is SHOW_VALUE
```

```
 T.W(SI)=2998.7724
POLY:Hit RETURN to continue
POLY: @@ A negative value means the temperature decreases
POLY: @@ if the amount is increased. Check for Mn
POLY:
POLY: s-c w(mn)
   ... the command in full is SET_CONDITION
Value /.0050000002/: .01
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         10854 grid points in             0 s
     9 ITS,  CPU TIME USED   0 SECONDS
POLY: sh t
   ... the command in full is SHOW_VALUE
 T=1058.8849
POLY:Hit RETURN to continue
POLY: @@ The temperature decreased from 1072 to 1059
POLY: @@ i.e. 13 degrees. According to the derivatives calculated
POLY: @@ above, you can increase the temperature the same
POLY: @@ amount by increasing the amount of Si
POLY: @@ 2592/2990=0.8669 times of the change in Mn
POLY: @@ i.e. from 0.3 to 0.733 %
POLY:
POLY: s-c w(si)
   ... the command in full is SET_CONDITION
Value /.003/: .00733
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         10854 grid points in             0 s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY: sh t
   ... the command in full is SHOW_VALUE
 T=1070.7315
POLY: @@ Being able to calculate these derivatives is a powerful
POLY: @@ feature in order to find the best way to obtain a
POLY: @@ specific property of a material.
POLY:
POLY: set-inter
   ... the command in full is SET_INTERACTIVE
POLY:
```

tcex19A

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex19A\tcex19A.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS:
SYS: @@ This is the first part of a two part example showing how
SYS: @@ to map univariant equilibria with the liquid in Al-Cu-Si.
SYS: @@ Part A. Step-by-step calculation using the POLY-3 module.
SYS:
SYS: set-log ex19a,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: 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
15:04:03,406 INFO  USER_1937707734_11, number of lines read: 470
15:04:04,865 INFO  Parsing of USER_1937707734_11 completed in 1565 ms
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
15:04:05,304 INFO  *** Invoking Gibbs Energy System v6 ***
 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

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
  'COST (1998): COST 507 -- Definition of Thermochemical and Thermophysical
      Properties to Provide a Database for the Development of New Light
      Alloys. European Cooperation in the Field of Scientific and Technical
      Research, European Commission. Vol 1. Proceedings of the Final
      Workshop of COST 507, Vaals, the Netherlands, 1997; Vol 2.
      Thermochemical Database for Light Metal Alloys (Eds. Ansara I.,
      Dinsdale A.T., and Rand M.H.); Vol 3. Critical Evaluation of Ternary
      Systems (Ed. Effenberg G.). '
 -OK-
TDB_USER: go p-3
```

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

 POLY version  3.32
POLY: s-c t=1300,p=101325,n=1
   ... the command in full is SET_CONDITION
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=1300, P=1.01325E5, N=1
 DEGREES OF FREEDOM 2
POLY: s-c x(si)=.25,x(al)=.2
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
15:04:08,145 INFO  Preparing system for use: USER_1937707734_11
15:04:09,152 INFO  Preparing phase for use: LIQUID
15:04:09,463 INFO  Preparing phase for use: ALCE_AMORPHOUS
15:04:09,612 INFO  Preparing phase for use: ALCUZN_T
15:04:09,757 INFO  Preparing phase for use: ALCU_DELTA
15:04:10,223 INFO  Preparing phase for use: ALCU_EPSILON
15:04:11,654 INFO  Preparing phase for use: ALCU_ETA
15:04:12,769 INFO  Preparing phase for use: ALCU_PRIME
15:04:12,923 INFO  Preparing phase for use: ALCU_THETA
15:04:13,199 INFO  Preparing phase for use: ALCU_ZETA
15:04:13,335 INFO  Preparing phase for use: ALLI
15:04:13,575 INFO  Preparing phase for use: ALMO
15:04:13,751 INFO  Preparing phase for use: ALM_D019
15:04:13,969 INFO  Preparing phase for use: ALND_AMORPHOUS
15:04:14,101 INFO  Preparing phase for use: ALTI
15:04:14,410 INFO  Preparing phase for use: BCC_B2
15:04:14,548 INFO  Preparing phase for use: BCC_A2
15:04:14,921 INFO  Preparing phase for use: BCT_A5
15:04:15,122 INFO  Preparing phase for use: CBCC_A12
15:04:15,304 INFO  Preparing phase for use: CR3SI_A15
15:04:15,441 INFO  Preparing phase for use: CRSI2
15:04:15,631 INFO  Preparing phase for use: CU19SI6_ETA
15:04:16,124 INFO  Preparing phase for use: CU33SI7_DELTA
15:04:16,471 INFO  Preparing phase for use: CU4SI_EPSILON
15:04:16,711 INFO  Preparing phase for use: CU56SI11_GAMMA
15:04:17,158 INFO  Preparing phase for use: CU6Y
15:04:17,277 INFO  Preparing phase for use: CUB_A13
15:04:17,995 INFO  Preparing phase for use: CUB_A15
15:04:18,209 INFO  Preparing phase for use: DIAMOND_A4
15:04:18,611 INFO  Preparing phase for use: FCC_A1
15:04:19,281 INFO  Preparing phase for use: GAMMA_D83
15:04:19,881 INFO  Preparing phase for use: GAMMA_H
15:04:20,395 INFO  Preparing phase for use: HCP_A3
15:04:20,534 INFO  Preparing phase for use: HCP_ZN
15:04:21,001 INFO  Preparing phase for use: LAVES_C14
15:04:21,143 INFO  Preparing phase for use: LAVES_C15
15:04:21,528 INFO  Preparing phase for use: LAVES_C36
15:04:21,713 INFO  Preparing phase for use: SIV3
Calculated         16744 grid points in             7 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     8  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: vwcs
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1300, P=1.01325E5, N=1, X(SI)=0.25, X(AL)=0.2
 DEGREES OF FREEDOM 0

 Temperature   1300.00 K (  1026.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.73680E+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:Hit RETURN to continue
POLY: @@ We want to calculate the monovariant lines with liquid.

POLY: @@ Select two compositions and the temperature as the axis.
POLY: 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: 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: s-a-v 3 t 500 2000 25
   ... the command in full is SET_AXIS_VARIABLE
POLY: @@ Set liquid as "present", otherwise all monovariant lines
POLY: @@ are calculated.
POLY: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: ?
 EQUILIBRIUM_CALCUL       NEW_COMPOSITION_SET      STABILITY_CHECK
 GLOBAL_MINIMIZATION      OUTPUT_FILE_FOR_SHOW     STEP_AND_MAP
 IGNORE_COMPOSI_SET_ORDER PARAEQUILIBRIUM          T-ZERO TEMPERATURE
 KEEP_COMP_SET_NUMBERS    PHASE_ADDITION           TOGGLE_ALTERNATE_MODE
 LIST_PHASE_ADDITION      PRESENT_PHASE
 MAJOR_CONSTITUENTS       SHOW_FOR_T=
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liquid
POLY:
POLY: save tcex19a1 y
   ... the command in full is SAVE_WORKSPACES
POLY: map
 Version R mapping is selected

 Organizing start points
```

```
NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point   1
Generating start point   2

Phase region boundary   1 at:   8.426E-02  2.500E-01  1.182E+03
    LIQUID
 ** BCC_B2
 ** DIAMOND_A4
*** Buffer saved on file:
c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex19A\tcex
19a1.POLY3
CALCULATED    35 EQUILIBRIA

Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
    LIQUID
    ALCU_EPSILON
 ** BCC_B2
 ** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
    LIQUID
 ** ALCU_EPSILON
 ** BCC_B2
Terminating at diagram limit
CALCULATED    18 EQUILIBRIA

Phase region boundary   2 at:   4.045E-01  1.269E-01  9.785E+02
    LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4
CALCULATED    20 EQUILIBRIA

Phase region boundary   2 at:   5.755E-01  8.764E-02  8.678E+02
    LIQUID
 ** ALCU_EPSILON
    ALCU_ETA
 ** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   5.755E-01  8.764E-02  8.678E+02
    LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA
Terminating at diagram limit
CALCULATED    16 EQUILIBRIA

Phase region boundary   2 at:   5.755E-01  8.764E-02  8.678E+02
    LIQUID
 ** ALCU_ETA
 ** DIAMOND_A4
CALCULATED     8 EQUILIBRIA

Phase region boundary   2 at:   6.299E-01  7.685E-02  8.291E+02
    LIQUID
 ** ALCU_ETA
    ALCU_THETA
 ** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   6.299E-01  7.685E-02  8.291E+02
    LIQUID
 ** ALCU_ETA
 ** ALCU_THETA
Terminating at diagram limit
CALCULATED    13 EQUILIBRIA

Phase region boundary   2 at:   6.299E-01  7.685E-02  8.291E+02
    LIQUID
 ** ALCU_THETA
 ** DIAMOND_A4
CALCULATED    18 EQUILIBRIA

Phase region boundary   2 at:   7.774E-01  7.282E-02  7.852E+02
    LIQUID
 ** ALCU_THETA
 ** DIAMOND_A4
    FCC_A1
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   7.774E-01  7.282E-02  7.852E+02
    LIQUID
 ** ALCU_THETA
 ** FCC_A1
Terminating at diagram limit
CALCULATED    12 EQUILIBRIA

Phase region boundary   2 at:   7.774E-01  7.282E-02  7.852E+02
    LIQUID
 ** DIAMOND_A4
 ** FCC_A1
*** SORRY CANNOT CONTINUE ***    4

CALCULATED    18 EQUILIBRIA

Phase region boundary   2 at:   8.426E-02  2.500E-01  1.182E+03
    LIQUID
 ** BCC_B2
 ** DIAMOND_A4
CALCULATED     8 EQUILIBRIA

Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
    LIQUID
 ** BCC_B2
    CU19SI6_ETA
 ** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
    LIQUID
 ** BCC_B2
 ** CU19SI6_ETA
Terminating at diagram limit
CALCULATED    12 EQUILIBRIA

Phase region boundary   2 at:   3.577E-02  2.616E-01  1.025E+03
```

```
     LIQUID
  ** CU19SI6_ETA
  ** DIAMOND_A4
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex19A\tcex19a1.POLY3
 CPU time for mapping                     1 seconds
POLY:
POLY: @@ The monovariant line FCC/BCC/LIQ in the Cu corner is not
POLY: @@ connected, so add a start point. This is different from a
POLY: @@ MAP with two axes, where all connected or non-connected
POLY: @@ lines can be found automatically.
POLY:
POLY: read tcex19a1
   ... the command in full is READ_WORKSPACES
POLY:
POLY: s-c x(al)=.1 x(si)=.1
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16744 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: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY:
POLY: map
 Version R mapping is selected

 Organizing start points

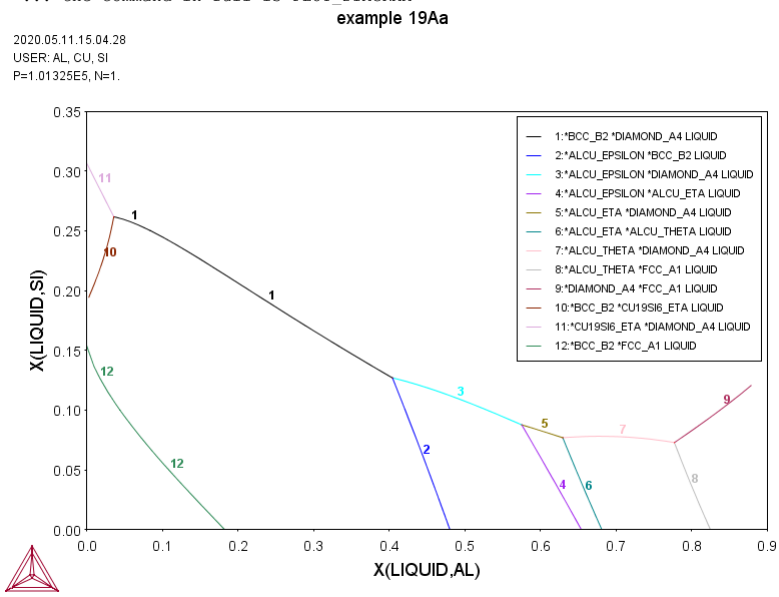
 NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.390E-02  1.000E-01  1.285E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED    18 EQUILIBRIA

 Phase region boundary   2 at:   4.390E-02  1.000E-01  1.285E+03
     LIQUID
  ** BCC_B2
  ** FCC_A1
 Terminating at diagram limit
 CALCULATED     9 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex19A\tcex19a1.POLY3
 CPU time for mapping                     0 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

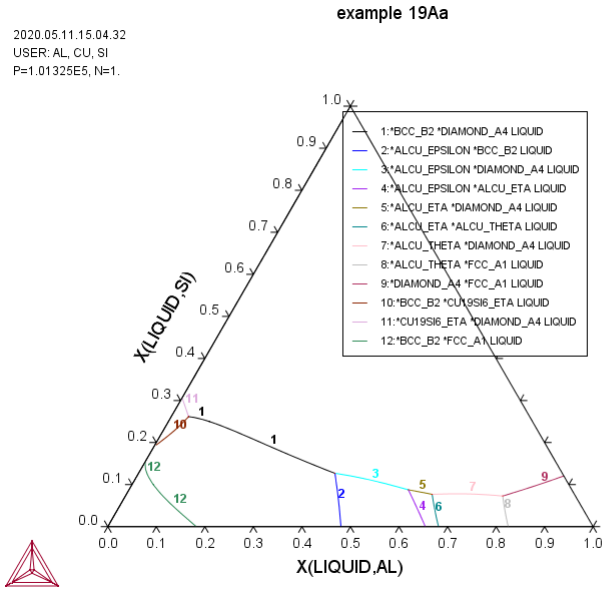
 Setting automatic diagram axes

POST: @@ We want the liquid compositions only
POST: s-d-a x x(liquid,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liquid,si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 19Aa
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

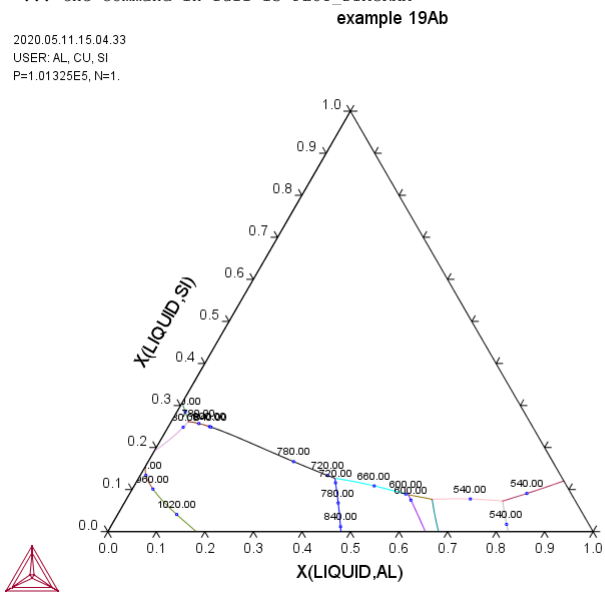



```
POST:
POST:Hit RETURN to continue
POST: @@ Make it triangular and scale the axis
POST: s-d-t
   ... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM  (Y OR N) /N/: y,,,,,,
```

```
POST: s-sc y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-sc x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: @@ Plot the phases stable along the lines
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Take away the phase labels and add tic
POST: @@ marks along the lines (the Z axis)
POST:
POST: s-lab n
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a z t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-sc z n 500 1000
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 19Ab
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Make a new calculation to overlay the monovariant
POST: @@ lines with isothermal calculations
POST:
POST: make tcex19a y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY: read tcex19a1
   ... the command in full is READ_WORKSPACES
```

```
POLY:
POLY: s-a-v 3
   ... the command in full is SET_AXIS_VARIABLE
Condition /T/: none
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16744 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: save tcex19a2 y
   ... the command in full is SAVE_WORKSPACES
POLY: 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: s-c x(al)
   ... the command in full is SET_CONDITION
Value /.2/: .10
POLY: @@ Use ADD to have several start points at different
POLY: @@ temperatures. But do not use default direction as
POLY: @@ that creates many start points. Increasing the Si
POLY: @@ content makes a solid phase stable.
POLY:
POLY: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: @@ You can have initial equilibria for different conditions
POLY: @@ at the same time. Just the axis variables have to be
POLY: @@ the same. To make nice isothermal curves is not easy;
POLY: @@  try with several start points to find all curve sections.
POLY:
POLY: s-c t
   ... the command in full is SET_CONDITION
Value /1300/: 1200
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16744 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: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: s-c t
   ... the command in full is SET_CONDITION
Value /1200/: 1100
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16744 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: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: @@ This line exists only in the Al rich corner
POLY: s-c x(al)=.5 x(si)=.1
   ... the command in full is SET_CONDITION
POLY: s-c t
   ... the command in full is SET_CONDITION
Value /1100/: 1000
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16744 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: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY: add 2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY: @@ A start point in the low melting Al corner too
POLY:
POLY: s-c x(al)=.9 x(si)=.01 t=900
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         16744 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: adva
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
```

```
POLY: add 1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

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

 Phase region boundary   1 at:   5.000E-02  6.891E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      10 equilibria

 Phase region boundary   2 at:   5.000E-02  6.891E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      52 equilibria

 Phase region boundary   3 at:   1.004E-01  3.055E-02
     LIQUID
  ** FCC_A1
 Calculated                      21 equilibria

 Phase region boundary   4 at:   1.004E-01  3.055E-02
     LIQUID
  ** FCC_A1
 Calculated.                      5 equilibria

 Phase region boundary   5 at:   1.373E-01  1.932E-02
     LIQUID
  ** BCC_B2
  ** FCC_A1

 Phase region boundary   6 at:   1.463E-01  2.848E-02
     LIQUID
  ** BCC_B2
 Calculated                      51 equilibria

 Phase region boundary   7 at:   1.373E-01  1.932E-02
     LIQUID
  ** FCC_A1
 Calculated                      27 equilibria

 Phase region boundary   8 at:   5.000E-02  6.515E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      43 equilibria

 Phase region boundary   9 at:   5.000E-02  6.515E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      52 equilibria

 Phase region boundary  10 at:   1.081E-01  1.639E-01
     LIQUID
  ** BCC_B2
 Calculated.                      16 equilibria

 Phase region boundary  11 at:   2.872E-02  1.169E-01
     LIQUID
  ** BCC_B2
  ** FCC_A1

 Phase region boundary  12 at:   2.764E-02  9.624E-02
     LIQUID
  ** FCC_A1
 Calculated                      13 equilibria

 Phase region boundary  13 at:   2.872E-02  1.169E-01
     LIQUID
  ** BCC_B2
 Calculated                      70 equilibria

 Phase region boundary  14 at:   1.081E-01  1.639E-01
     LIQUID
  ** BCC_B2
 Calculated                      44 equilibria

 Phase region boundary  15 at:   5.000E-02  6.262E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      38 equilibria

 Phase region boundary  16 at:   5.000E-02  6.262E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      56 equilibria
```

```
Phase region boundary  17 at:   1.116E-01  1.999E-01
    LIQUID
 ** BCC_B2
Calculated                     23 equilibria

Phase region boundary  18 at:   1.116E-01  1.999E-01
    LIQUID
 ** BCC_B2
Calculated.                     34 equilibria

Phase region boundary  19 at:   4.370E-01  1.765E-02
    LIQUID
 ** ALCU_EPSILON
 ** BCC_B2

Phase region boundary  20 at:   4.453E-01  1.265E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                     18 equilibria

Phase region boundary  21 at:   4.370E-01  1.765E-02
    LIQUID
 ** BCC_B2
Calculated.                     43 equilibria

Phase region boundary  22 at:   2.106E-02  1.939E-01
    LIQUID
 ** BCC_B2
 ** CU19SI6_ETA

Phase region boundary  23 at:   7.190E-03  2.263E-01
    LIQUID
 ** CU19SI6_ETA
Calculated                     24 equilibria

Phase region boundary  24 at:   2.500E-01  5.691E-01
    LIQUID
 ** DIAMOND_A4
Calculated.                      8 equilibria

Phase region boundary  25 at:   1.890E-01  5.683E-01
    LIQUID
 ** BCC_B2
 ** DIAMOND_A4

Phase region boundary  26 at:   3.667E-01  1.003E-01
    LIQUID
 ** BCC_B2
Calculated.                      5 equilibria

Phase region boundary  27 at:   3.979E-01  7.953E-02
    LIQUID
 ** ALCU_EPSILON
 ** BCC_B2

Phase region boundary  28 at:   4.219E-01  5.542E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                     28 equilibria

Phase region boundary  29 at:   1.890E-01  5.683E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     42 equilibria

Phase region boundary  30 at:   2.500E-01  5.691E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     49 equilibria

Phase region boundary  31 at:   4.698E-01  3.348E-02
    LIQUID
 ** ALCU_EPSILON
Calculated.                      6 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   4.698E-01  3.348E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                     27 equilibria

Phase region boundary  33 at:   9.694E-01  5.516E-03
    LIQUID
 ** FCC_A1
Calculated                     12 equilibria

Phase region boundary  34 at:   9.694E-01  5.516E-03
    LIQUID
 ** FCC_A1
Calculated                     16 equilibria

Phase region boundary  35 at:   5.506E-01  5.000E-03
    LIQUID
 ** ALCU_EPSILON
Calculated                     18 equilibria

Phase region boundary  36 at:   5.506E-01  5.000E-03
    LIQUID
 ** ALCU_EPSILON
Calculated.                     10 equilibria

Phase region boundary  37 at:   4.954E-01  4.888E-02
    LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4

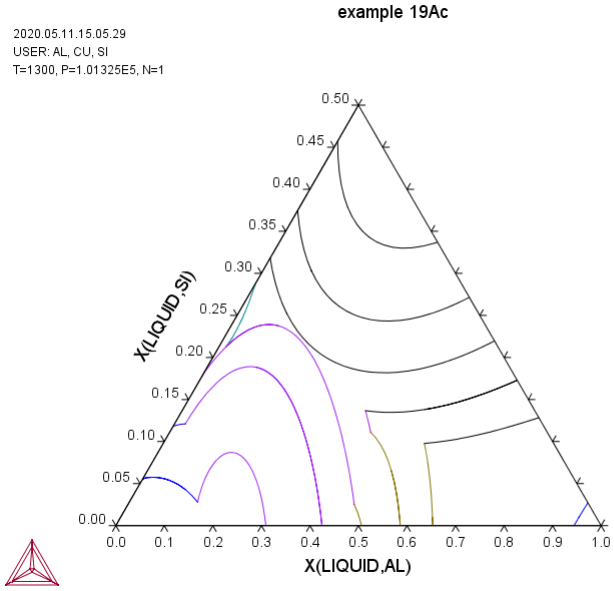
Phase region boundary  38 at:   2.690E-01  5.489E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     35 equilibria

Phase region boundary  39 at:   4.954E-01  4.888E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                     22 equilibria
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex19A\tcex19a2.POLY3
```

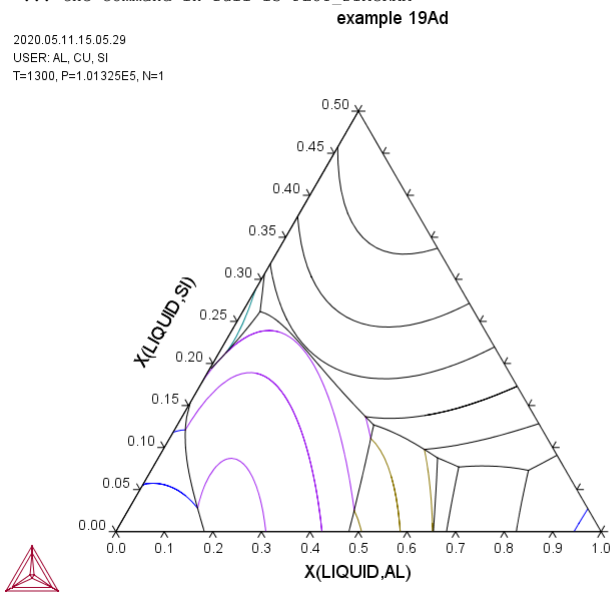
```
 CPU time for mapping                    10 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x x(liquid,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liquid,si)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST:
POST:
POST: set-title example 19Ac
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

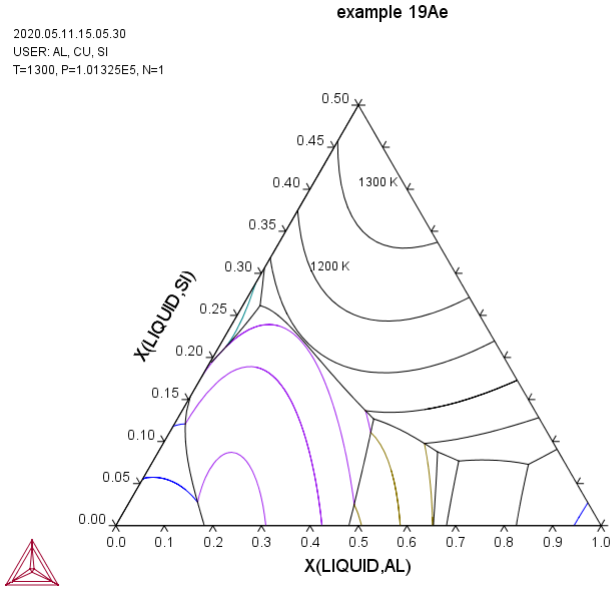



```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex19a
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 19Ad
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: add .1 .4 n 1300 K
   ... the command in full is ADD_LABEL_TEXT
Text size: /.36/:
POST:
POST: add .1 .3 n 1200 K
```

```
   ... the command in full is ADD_LABEL_TEXT
Text size: /.36/:
POST:
POST: set-title example 19Ae
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex19B

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex19B\tcex19B.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS:
SYS: @@ This is the second part of a two part example showing how
SYS: @@ to map univariant equilibria with the liquid in Al-Cu-Si.
SYS: @@ Part B. Using the Ternary module, you can get the
SYS: @@ information on invariant reactions, such as temperature
SYS: @@ 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
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
 Current database: Iron Demo Database v3.0

 VA                      /-  DEFINED
Database: /FEDEMO/: user tcex19_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
15:07:02,093 INFO  USER_1360187209_11, number of lines read: 470
15:07:03,603 INFO  Parsing of USER_1360187209_11 completed in 1604 ms
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 GES .....
 AL                      CU                      SI
   DEFINED
 *** ERROR GAS INPUT IGNORED

 ************************************************************
 * WARNING: This database has no list of assessed systems *
 *             The diagram may be wrong.                  *
 ************************************************************

Quit? /Y/: N
15:07:03,858 INFO  *** Invoking Gibbs Energy System v6 ***
 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

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
  'COST (1998): COST 507 -- Definition of Thermochemical and Thermophysical
      Properties to Provide a Database for the Development of New Light
      Alloys. European Cooperation in the Field of Scientific and Technical
      Research, European Commission. Vol 1. Proceedings of the Final
      Workshop of COST 507, Vaals, the Netherlands, 1997; Vol 2.
      Thermochemical Database for Light Metal Alloys (Eds. Ansara I.,
      Dinsdale A.T., and Rand M.H.); Vol 3. Critical Evaluation of Ternary
      Systems (Ed. Effenberg G.). '
 -OK-
 Forcing automatic start values
 Automatic start values will be set
15:07:05,250 INFO  Preparing system for use: USER_1360187209_11
15:07:06,325 INFO  Preparing phase for use: LIQUID
15:07:06,545 INFO  Preparing phase for use: ALCE_AMORPHOUS
15:07:06,666 INFO  Preparing phase for use: ALCUZN_T
15:07:06,800 INFO  Preparing phase for use: ALCU_DELTA
15:07:06,943 INFO  Preparing phase for use: ALCU_EPSILON
15:07:07,057 INFO  Preparing phase for use: ALCU_ETA
15:07:07,188 INFO  Preparing phase for use: ALCU_PRIME
15:07:07,283 INFO  Preparing phase for use: ALCU_THETA
15:07:07,405 INFO  Preparing phase for use: ALCU_ZETA
15:07:07,511 INFO  Preparing phase for use: ALLI
15:07:07,618 INFO  Preparing phase for use: ALMO
15:07:07,722 INFO  Preparing phase for use: ALM_D019
15:07:07,827 INFO  Preparing phase for use: ALND_AMORPHOUS
15:07:07,988 INFO  Preparing phase for use: ALTI
15:07:08,106 INFO  Preparing phase for use: BCC_B2
15:07:08,209 INFO  Preparing phase for use: BCC_A2
15:07:08,307 INFO  Preparing phase for use: BCT_A5
15:07:08,409 INFO  Preparing phase for use: CBCC_A12
15:07:08,508 INFO  Preparing phase for use: CR3SI_A15
```

```
15:07:08,615 INFO  Preparing phase for use: CRSI2
15:07:08,709 INFO  Preparing phase for use: CU19SI6_ETA
15:07:08,933 INFO  Preparing phase for use: CU33SI7_DELTA
15:07:09,027 INFO  Preparing phase for use: CU4SI_EPSILON
15:07:09,160 INFO  Preparing phase for use: CU56SI11_GAMMA
15:07:09,248 INFO  Preparing phase for use: CU6Y
15:07:09,423 INFO  Preparing phase for use: CUB_A13
15:07:09,922 INFO  Preparing phase for use: CUB_A15
15:07:10,111 INFO  Preparing phase for use: DIAMOND_A4
15:07:10,339 INFO  Preparing phase for use: FCC_A1
15:07:10,521 INFO  Preparing phase for use: GAMMA_D83
15:07:10,786 INFO  Preparing phase for use: GAMMA_H
15:07:10,941 INFO  Preparing phase for use: HCP_A3
15:07:11,052 INFO  Preparing phase for use: HCP_ZN
15:07:11,201 INFO  Preparing phase for use: LAVES_C14
15:07:11,294 INFO  Preparing phase for use: LAVES_C15
15:07:11,402 INFO  Preparing phase for use: LAVES_C36
15:07:11,506 INFO  Preparing phase for use: SIV3
 Forcing automatic start values
 Automatic start values will be set
 Forcing automatic start values
 Automatic start values will be set

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

 T = 1673.15 K
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   7.327E-03  9.853E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     15 equilibria

 Phase region boundary   2 at:   7.327E-03  9.853E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     15 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                      2 seconds
 T = 1573.15 K

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   7.453E-02  8.883E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     23 equilibria

 Phase region boundary   2 at:   7.453E-02  8.883E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     25 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                      0 seconds
 T = 1473.15 K

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   1.372E-01  7.942E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     30 equilibria

 Phase region boundary   2 at:   1.372E-01  7.942E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     22 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                      1 seconds
 T = 1373.15 K

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   1.926E-01  7.111E-01
```

```
     LIQUID
  ** DIAMOND_A4
 Calculated                      28 equilibria

 Phase region boundary   2 at:   1.926E-01  7.111E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      32 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                       1 seconds
 T = 1273.15 K

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   6.652E-01  9.329E-03
     LIQUID
  ** BCC_B2
 Calculated.                      2 equilibria

 Phase region boundary   2 at:   6.645E-01  6.795E-03
     LIQUID
  ** BCC_B2
  ** GAMMA_H

 Phase region boundary   3 at:   6.653E-01  4.077E-03
     LIQUID
  ** GAMMA_H
 Calculated                      12 equilibria

 Phase region boundary   4 at:   6.645E-01  6.795E-03
     LIQUID
  ** BCC_B2
 Calculated.                      29 equilibria

 Phase region boundary   5 at:   8.419E-01  6.666E-02
     LIQUID
  ** BCC_B2
  ** FCC_A1

 Phase region boundary   6 at:   8.633E-01  4.917E-02
     LIQUID
  ** FCC_A1
 Calculated                      25 equilibria

 Phase region boundary   7 at:   6.652E-01  9.329E-03
     LIQUID
  ** BCC_B2
 Calculated.                      30 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                       1 seconds

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   2.311E-01  6.535E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      34 equilibria

 Phase region boundary   2 at:   2.311E-01  6.535E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      34 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                       0 seconds
 T = 1173.15 K

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   5.840E-01  7.591E-03
     LIQUID
  ** BCC_B2
 Calculated                      9 equilibria

 Phase region boundary   2 at:   5.840E-01  7.591E-03
     LIQUID
  ** BCC_B2
 Calculated.                      39 equilibria

 Phase region boundary   3 at:   8.543E-01  1.296E-01
     LIQUID
  ** BCC_B2
  ** FCC_A1
```

```
 Phase region boundary   4 at:   8.749E-01  1.099E-01
     LIQUID
  ** FCC_A1
 Calculated                     24 equilibria

 Phase region boundary   5 at:   8.543E-01  1.296E-01
     LIQUID
  ** BCC_B2
 Calculated                     54 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                     2 seconds

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   2.562E-01  6.158E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     39 equilibria

 Phase region boundary   2 at:   2.562E-01  6.158E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     37 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                     1 seconds
 T = 1073.15 K

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   5.198E-01  5.412E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated                     11 equilibria

 Phase region boundary   2 at:   5.198E-01  5.412E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated.                     5 equilibria

 Phase region boundary   3 at:   5.361E-01  2.533E-02
     LIQUID
  ** ALCU_EPSILON
  ** BCC_B2

 Phase region boundary   4 at:   5.383E-01  3.569E-02
     LIQUID
  ** BCC_B2
 Calculated.                     12 equilibria

 Phase region boundary   5 at:   5.962E-01  1.431E-01
     LIQUID
  ** BCC_B2
  ** DIAMOND_A4

 Phase region boundary   6 at:   2.789E-01  5.911E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                     41 equilibria

 Phase region boundary   7 at:   5.361E-01  2.533E-02
     LIQUID
  ** ALCU_EPSILON
 Calculated                     16 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                     0 seconds

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   7.337E-01  2.597E-01
     LIQUID
  ** CU19SI6_ETA
 Calculated.                     4 equilibria

 Phase region boundary   2 at:   7.478E-01  2.387E-01
     LIQUID
  ** BCC_B2
  ** CU19SI6_ETA

 Phase region boundary   3 at:   7.525E-01  2.105E-01
     LIQUID
  ** BCC_B2
 Calculated.                     8 equilibria
```

```
 Phase region boundary   4 at:   6.917E-01  2.112E-01
     LIQUID
  ** BCC_B2
  ** DIAMOND_A4

 Phase region boundary   5 at:   3.329E-01  6.250E-01
     LIQUID
  ** DIAMOND_A4
 Calculated.                      14 equilibria

 Phase region boundary   6 at:   3.469E-01  6.529E-01
     LIQUID
  ** CU19SI6_ETA
  ** DIAMOND_A4

 Phase region boundary   7 at:   7.269E-01  2.729E-01
     LIQUID
  ** CU19SI6_ETA
 Calculated.                       6 equilibria
 Terminating at known equilibrium

 Phase region boundary   8 at:   7.337E-01  2.597E-01
     LIQUID
  ** CU19SI6_ETA
 Calculated.                       3 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                     0 seconds
 T =  973.15 K

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.736E-01  5.113E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated                      12 equilibria

 Phase region boundary   2 at:   4.736E-01  5.113E-03
     LIQUID
  ** ALCU_EPSILON
 Calculated.                      11 equilibria

 Phase region boundary   3 at:   5.106E-01  6.209E-02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4

 Phase region boundary   4 at:   2.273E-01  5.621E-01
     LIQUID
  ** DIAMOND_A4
 Calculated                      36 equilibria

 Phase region boundary   5 at:   5.106E-01  6.209E-02
     LIQUID
  ** ALCU_EPSILON
 Calculated                      24 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                     1 seconds
 T =  873.15 K

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   3.646E-02  1.803E-02
     LIQUID
  ** FCC_A1
 Calculated                      15 equilibria

 Phase region boundary   2 at:   3.646E-02  1.803E-02
     LIQUID
  ** FCC_A1
 Calculated                      33 equilibria
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
 CPU time for mapping                     0 seconds

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

 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   4.151E-01  5.493E-03
     LIQUID
  ** ALCU_ETA
 Calculated                       8 equilibria

 Phase region boundary   2 at:   4.151E-01  5.493E-03
```

```
     LIQUID
 ** ALCU_ETA
Calculated.                      6 equilibria

Phase region boundary   3 at:   4.241E-01  3.756E-02
     LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA

Phase region boundary   4 at:   4.398E-01  3.756E-02
     LIQUID
 ** ALCU_EPSILON
Calculated.                      2 equilibria

Phase region boundary   5 at:   4.420E-01  4.464E-02
     LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4

Phase region boundary   6 at:   1.706E-01  5.446E-01
     LIQUID
 ** DIAMOND_A4
Calculated                     27 equilibria

Phase region boundary   7 at:   4.241E-01  3.756E-02
     LIQUID
 ** ALCU_ETA
Calculated                     17 equilibria
*** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping                     1 seconds
T =  773.15 K

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

T = 1773.15 K
Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point   1
Generating start point   2

Phase region boundary   1 at:   3.379E-01  7.512E-02  8.731E+02
     LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA
CALCULATED     4 EQUILIBRIA

Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA
     DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4
CALCULATED    25 EQUILIBRIA

Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
 ** ALCU_EPSILON
     BCC_B2
 ** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
 ** ALCU_EPSILON
 ** BCC_B2
Terminating at diagram limit
CALCULATED    34 EQUILIBRIA

Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
 ** BCC_B2
 ** DIAMOND_A4
CALCULATED    43 EQUILIBRIA

Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
 ** BCC_B2
     CU19SI6_ETA
 ** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
 ** BCC_B2
 ** CU19SI6_ETA
Terminating at known equilibrium
CALCULATED    37 EQUILIBRIA

Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
 ** CU19SI6_ETA
 ** DIAMOND_A4
*** SORRY CANNOT CONTINUE ***    4

CALCULATED    16 EQUILIBRIA

Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
 ** ALCU_ETA
 ** DIAMOND_A4
CALCULATED     9 EQUILIBRIA

Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
 ** ALCU_ETA
```

```
     ALCU_THETA
 ** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
 ** ALCU_ETA
 ** ALCU_THETA
Terminating at diagram limit
CALCULATED    14 EQUILIBRIA

Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
 ** ALCU_THETA
 ** DIAMOND_A4
CALCULATED    17 EQUILIBRIA

Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
     LIQUID
 ** ALCU_THETA
 ** DIAMOND_A4
     FCC_A1
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
     LIQUID
 ** ALCU_THETA
 ** FCC_A1
Terminating at diagram limit
CALCULATED    12 EQUILIBRIA

Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
     LIQUID
 ** DIAMOND_A4
 ** FCC_A1
Terminating at diagram limit
CALCULATED    21 EQUILIBRIA

Phase region boundary   2 at:   3.379E-01  7.512E-02  8.731E+02
     LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA
Terminating at diagram limit
CALCULATED    12 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\LIQUIDUS_002.POLY3
CPU time for mapping                     1 seconds

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

Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point   1
Generating start point   2

Phase region boundary   1 at:   8.482E-01  6.736E-02  1.273E+03
     LIQUID
 ** BCC_B2
 ** FCC_A1
*** SORRY CANNOT CONTINUE ***    9

CALCULATED    46 EQUILIBRIA

Phase region boundary   2 at:   8.482E-01  6.736E-02  1.273E+03
     LIQUID
 ** BCC_B2
 ** FCC_A1
Terminating at diagram limit
CALCULATED    13 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\LIQUIDUS_002.POLY3
CPU time for mapping                     0 seconds

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

Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point   1
Generating start point   2

Phase region boundary   1 at:   6.503E-01  8.154E-03  1.273E+03
     LIQUID
 ** BCC_B2
 ** GAMMA_H
Terminating at diagram limit
CALCULATED    13 EQUILIBRIA

Phase region boundary   2 at:   6.503E-01  8.154E-03  1.273E+03
     LIQUID
 ** BCC_B2
 ** GAMMA_H
Terminating at diagram limit
CALCULATED     9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\LIQUIDUS_002.POLY3
CPU time for mapping                     0 seconds
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
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 Automatic start values will be set
 Forcing automatic start values
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 Forcing automatic start values
 Automatic start values will be set

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

 Version R mapping is selected

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6

 Phase region boundary   1 at:   3.379E-01  7.512E-02  8.731E+02
     LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA
 CALCULATED     4 EQUILIBRIA

 Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA
     DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4
 CALCULATED    25 EQUILIBRIA

 Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
  ** ALCU_EPSILON
     BCC_B2
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
  ** ALCU_EPSILON
  ** BCC_B2
 Terminating at diagram limit
 CALCULATED    34 EQUILIBRIA

 Phase region boundary   2 at:   4.686E-01  1.269E-01  9.785E+02
     LIQUID
  ** BCC_B2
  ** DIAMOND_A4
 CALCULATED    43 EQUILIBRIA

 Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
  ** BCC_B2
     CU19SI6_ETA
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
  ** BCC_B2
  ** CU19SI6_ETA
 Terminating at known equilibrium
 CALCULATED    37 EQUILIBRIA

 Phase region boundary   2 at:   7.026E-01  2.616E-01  1.025E+03
     LIQUID
  ** CU19SI6_ETA
  ** DIAMOND_A4
 *** SORRY CANNOT CONTINUE ***    4

 CALCULATED    16 EQUILIBRIA

 Phase region boundary   2 at:   3.369E-01  8.764E-02  8.678E+02
     LIQUID
  ** ALCU_ETA
  ** DIAMOND_A4
 CALCULATED     9 EQUILIBRIA

 Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
  ** ALCU_ETA
     ALCU_THETA
  ** DIAMOND_A4
 SKIPPING LINE WITHOUT LIQUID#1

 Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
  ** ALCU_ETA
  ** ALCU_THETA
 Terminating at diagram limit
 CALCULATED    14 EQUILIBRIA

 Phase region boundary   2 at:   2.933E-01  7.685E-02  8.291E+02
     LIQUID
```

```
 ** ALCU_THETA
 ** DIAMOND_A4
CALCULATED    17 EQUILIBRIA

Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
    LIQUID
 ** ALCU_THETA
 ** DIAMOND_A4
    FCC_A1
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
    LIQUID
 ** ALCU_THETA
 ** FCC_A1
Terminating at diagram limit
CALCULATED    12 EQUILIBRIA

Phase region boundary   2 at:   1.498E-01  7.282E-02  7.852E+02
    LIQUID
 ** DIAMOND_A4
 ** FCC_A1
Terminating at diagram limit
CALCULATED    21 EQUILIBRIA

Phase region boundary   2 at:   3.379E-01  7.512E-02  8.731E+02
    LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA
Terminating at diagram limit
CALCULATED    12 EQUILIBRIA

Phase region boundary   2 at:   8.482E-01  6.736E-02  1.273E+03
    LIQUID
 ** BCC_B2
 ** FCC_A1
*** SORRY CANNOT CONTINUE ***    9

CALCULATED    46 EQUILIBRIA

Phase region boundary   2 at:   8.482E-01  6.736E-02  1.273E+03
    LIQUID
 ** BCC_B2
 ** FCC_A1
Terminating at diagram limit
CALCULATED    13 EQUILIBRIA

Phase region boundary   2 at:   6.503E-01  8.154E-03  1.273E+03
    LIQUID
 ** BCC_B2
 ** GAMMA_H
Terminating at diagram limit
CALCULATED    13 EQUILIBRIA

Phase region boundary   2 at:   6.503E-01  8.154E-03  1.273E+03
    LIQUID
 ** BCC_B2
 ** GAMMA_H
Terminating at diagram limit
CALCULATED     9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping                     1 seconds
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
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Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

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

```
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28
Generating start point  29
Generating start point  30
Generating start point  31
Generating start point  32
Generating start point  33
Generating start point  34
Generating start point  35
Working hard

Phase region boundary   1 at:   4.398E-01  3.756E-02
    LIQUID
 ** ALCU_EPSILON
Calculated.                      2 equilibria

Phase region boundary   2 at:   4.420E-01  4.464E-02
    LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4

Phase region boundary   3 at:   1.706E-01  5.446E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     30 equilibria

Phase region boundary   4 at:   4.420E-01  4.464E-02
    LIQUID
 ** ALCU_EPSILON
Calculated.                      2 equilibria

Phase region boundary   5 at:   4.398E-01  3.756E-02
    LIQUID
 ** ALCU_EPSILON
 ** ALCU_ETA

Phase region boundary   6 at:   4.241E-01  3.756E-02
    LIQUID
 ** ALCU_ETA
Calculated                     19 equilibria

Phase region boundary   7 at:   4.241E-01  3.756E-02
    LIQUID
 ** ALCU_ETA
Calculated                     19 equilibria

Phase region boundary   8 at:   8.419E-01  6.666E-02
    LIQUID
 ** BCC_B2
Calculated.                      1 equilibria

Phase region boundary   9 at:   8.419E-01  6.666E-02
    LIQUID
 ** BCC_B2
 ** FCC_A1

Phase region boundary  10 at:   8.633E-01  4.917E-02
    LIQUID
 ** FCC_A1
Calculated                     25 equilibria

Phase region boundary  11 at:   8.419E-01  6.666E-02
    LIQUID
 ** BCC_B2
Calculated.                     28 equilibria

Phase region boundary  12 at:   6.645E-01  6.795E-03
    LIQUID
 ** BCC_B2
 ** GAMMA_H

Phase region boundary  13 at:   6.653E-01  4.077E-03
    LIQUID
 ** GAMMA_H
Calculated                     12 equilibria

Phase region boundary  14 at:   8.633E-01  4.917E-02
    LIQUID
 ** FCC_A1
Calculated                     25 equilibria

Phase region boundary  15 at:   6.645E-01  6.795E-03
    LIQUID
 ** BCC_B2
Calculated.                     26 equilibria
Terminating at known equilibrium

Phase region boundary  16 at:   6.653E-01  4.077E-03
    LIQUID
 ** GAMMA_H
Calculated.                      1 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.327E-03  9.853E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     15 equilibria

Phase region boundary  18 at:   7.327E-03  9.853E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     15 equilibria

Phase region boundary  19 at:   7.453E-02  8.883E-01
    LIQUID
 ** DIAMOND_A4
Calculated                     23 equilibria

Phase region boundary  20 at:   7.453E-02  8.883E-01
    LIQUID
```

```
 ** DIAMOND_A4
Calculated                      25 equilibria

Phase region boundary  21 at:   1.372E-01  7.942E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      30 equilibria

Phase region boundary  22 at:   1.372E-01  7.942E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      22 equilibria

Phase region boundary  23 at:   1.926E-01  7.111E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      28 equilibria

Phase region boundary  24 at:   1.926E-01  7.111E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      32 equilibria

Phase region boundary  25 at:   6.652E-01  9.329E-03
    LIQUID
 ** BCC_B2
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  26 at:   6.652E-01  9.329E-03
    LIQUID
 ** BCC_B2
Calculated.                     30 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   2.311E-01  6.535E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      34 equilibria

Phase region boundary  28 at:   2.311E-01  6.535E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      40 equilibria

Phase region boundary  29 at:   5.840E-01  7.591E-03
    LIQUID
 ** BCC_B2
Calculated                       9 equilibria

Phase region boundary  30 at:   5.840E-01  7.591E-03
    LIQUID
 ** BCC_B2
Calculated.                     39 equilibria

Phase region boundary  31 at:   8.543E-01  1.296E-01
    LIQUID
 ** BCC_B2
 ** FCC_A1

Phase region boundary  32 at:   8.749E-01  1.099E-01
    LIQUID
 ** FCC_A1
Calculated                      24 equilibria

Phase region boundary  33 at:   8.543E-01  1.296E-01
    LIQUID
 ** BCC_B2
Calculated                      54 equilibria

Phase region boundary  34 at:   2.562E-01  6.158E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      39 equilibria

Phase region boundary  35 at:   2.562E-01  6.158E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      37 equilibria

Phase region boundary  36 at:   5.198E-01  5.412E-03
    LIQUID
 ** ALCU_EPSILON
Calculated                      11 equilibria

Phase region boundary  37 at:   5.198E-01  5.412E-03
    LIQUID
 ** ALCU_EPSILON
Calculated.                      5 equilibria

Phase region boundary  38 at:   5.361E-01  2.533E-02
    LIQUID
 ** ALCU_EPSILON
 ** BCC_B2

Phase region boundary  39 at:   5.383E-01  3.569E-02
    LIQUID
 ** BCC_B2
Calculated.                     12 equilibria

Phase region boundary  40 at:   5.962E-01  1.431E-01
    LIQUID
 ** BCC_B2
 ** DIAMOND_A4

Phase region boundary  41 at:   2.789E-01  5.911E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      41 equilibria

Phase region boundary  42 at:   5.361E-01  2.533E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                      16 equilibria

Phase region boundary  43 at:   7.337E-01  2.597E-01
```

```
    LIQUID
 ** CU19SI6_ETA
Calculated.                      4 equilibria

Phase region boundary  44 at:   7.478E-01  2.387E-01
    LIQUID
 ** BCC_B2
 ** CU19SI6_ETA

Phase region boundary  45 at:   7.525E-01  2.105E-01
    LIQUID
 ** BCC_B2
Calculated.                      8 equilibria

Phase region boundary  46 at:   6.917E-01  2.112E-01
    LIQUID
 ** BCC_B2
 ** DIAMOND_A4

Phase region boundary  47 at:   3.329E-01  6.250E-01
    LIQUID
 ** DIAMOND_A4
Calculated.                     14 equilibria

Phase region boundary  48 at:   3.469E-01  6.529E-01
    LIQUID
 ** CU19SI6_ETA
 ** DIAMOND_A4

Phase region boundary  49 at:   7.269E-01  2.729E-01
    LIQUID
 ** CU19SI6_ETA
Calculated.                      6 equilibria
Terminating at known equilibrium

Phase region boundary  50 at:   7.337E-01  2.597E-01
    LIQUID
 ** CU19SI6_ETA
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  51 at:   4.736E-01  5.113E-03
    LIQUID
 ** ALCU_EPSILON
Calculated                      12 equilibria

Phase region boundary  52 at:   4.736E-01  5.113E-03
    LIQUID
 ** ALCU_EPSILON
Calculated.                     11 equilibria

Phase region boundary  53 at:   5.106E-01  6.209E-02
    LIQUID
 ** ALCU_EPSILON
 ** DIAMOND_A4

Phase region boundary  54 at:   2.273E-01  5.621E-01
    LIQUID
 ** DIAMOND_A4
Calculated                      36 equilibria

Phase region boundary  55 at:   5.106E-01  6.209E-02
    LIQUID
 ** ALCU_EPSILON
Calculated                      24 equilibria

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: C:\Users\vagrant\AppData\Local\Temp\MONOVAR_002.POLY3
CPU time for mapping                    7 seconds
 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

 POSTPROCESSOR VERSION 3.2

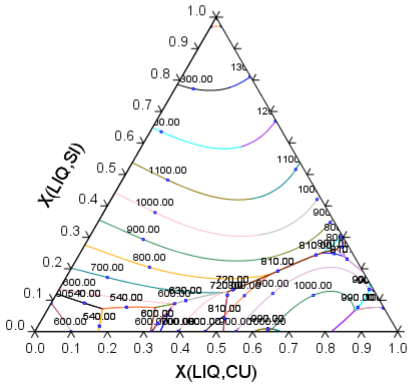
Setting automatic diagram axes


INVARIANT REACTIONS:

E 1:  751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1:  705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2:  594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3:  555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2:  512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1
```

AL-CU-SI (600C/1400C/100C)

2020.05.11.15.08.43
USER: AL, CU, SI
P=1E5, N=1



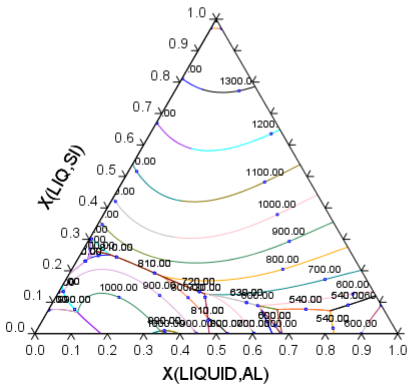
INVARIANT REACTIONS:

E 1 : 751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1 : 705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2 : 594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3 : 555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2 : 512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1

```
POST: s-d-a x x(liquid,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 19B
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

example 19B

2020.05.11.15.09.06
USER: AL, CU, SI
P=1E5, N=1



INVARIANT REACTIONS:

E 1 : 751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1 : 705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2 : 594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3 : 555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2 : 512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1

```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex20

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex20\tcex20.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Adiabatic decompression in a geological system
SYS:
SYS: @@ This example calculates the adiabatic decompression
SYS: @@ in a geological system using the geochemical
SYS: @@ database (PGEO.TDB)
SYS:
SYS: set-log ex20,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw user PGEO.TDB
   ... the command in full is SWITCH_DATABASE
 Current database: User defined Database

 O                       VA  DEFINED
 STEAM                   OXYGEN                  HYDROGEN
   REJECTED
 CARBON_MONOXIDE         CARBON_DIOXIDE          METHANE
   REJECTED
15:10:23,357 INFO  USER_1998433168_11, number of lines read: 3095
15:10:25,919 INFO  Parsing of USER_1998433168_11 completed in 2701 ms
TDB_USER: d-sys mg si
   ... the command in full is DEFINE_SYSTEM
 MG                      SI  DEFINED
TDB_USER: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
 GAS:G       :O2:
  > Gaseous Mixture with C-H-O species, using ideal gas model
 A_QUARTZ    :SI1O2:
 B_QUARTZ    :SI1O2:
 CRISTOBALITE :SI1O2:
 TRIDYMITE   :SI1O2:
 COESITE     :SI1O2:
 STISHOVITE  :SI1O2:
 PERICLASE   :MG1O1:
 FORSTERITE  :SI1MG2O4:
 BETA_FORSTERITE :SI1MG2O4:
 GAMMA_FORSTERITE :SI1MG2O4:
 ILMENITE_MG :SI1MG1O3:
 MG_PEROVSKITE :SI1MG1O3:
 CLINOENSTATITE :SI1MG1O3:
 ORTHOENSTATITE :SI1MG1O3:
 PROTOENSTATITE :SI1MG1O3:
 CLINOENSTHP :SI1MG1O3:
 GARNET_MG   :SI1MG1O3:
TDB_USER: rej ph gas proto
   ... the command in full is REJECT
 GAS:G                   PROTOENSTATITE  REJECTED
TDB_USER: get
   ... the command in full is GET_DATA
15:10:27,177 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ Define more convenient components

POLY: def-com mgo o sio2
   ... the command in full is DEFINE_COMPONENTS
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 MGO                     ENTERED   SER
 O                       ENTERED   SER
 SIO2                    ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 TRIDYMITE               ENTERED      0.000000E+00    0.000000E+00
 STISHOVITE              ENTERED      0.000000E+00    0.000000E+00
 PERICLASE               ENTERED      0.000000E+00    0.000000E+00
 ORTHOENSTATITE          ENTERED      0.000000E+00    0.000000E+00
 MG_PEROVSKITE           ENTERED      0.000000E+00    0.000000E+00
 ILMENITE_MG             ENTERED      0.000000E+00    0.000000E+00
 GARNET_MG               ENTERED      0.000000E+00    0.000000E+00
 GAMMA_FORSTERITE        ENTERED      0.000000E+00    0.000000E+00
 FORSTERITE              ENTERED      0.000000E+00    0.000000E+00
 CRISTOBALITE            ENTERED      0.000000E+00    0.000000E+00
 COESITE                 ENTERED      0.000000E+00    0.000000E+00
 CLINOENSTHP             ENTERED      0.000000E+00    0.000000E+00
```

```
 CLINOENSTATITE          ENTERED      0.000000E+00    0.000000E+00
 B_QUARTZ                ENTERED      0.000000E+00    0.000000E+00
 BETA_FORSTERITE         ENTERED      0.000000E+00    0.000000E+00
 A_QUARTZ                ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 MG       ENTERED    O        ENTERED    SI1MG1O3 ENTERED    SIO2     ENTERED
 MG1O1    ENTERED    O2       ENTERED    SI1MG2O4 ENTERED    VA       ENTERED
 MGO      ENTERED    SI       ENTERED    SI1O2    ENTERED
POLY:Hit RETURN to continue
POLY: @@ and specify a composition assumed
POLY: @@ to be present in the Earth's mantle
POLY:
POLY: s-i-a n(mgo)=80
   ... the command in full is SET_INPUT_AMOUNTS
POLY: s-i-a n(si1mg1o3)=100
   ... the command in full is SET_INPUT_AMOUNTS
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 N(MGO)=180, N(SIO2)=100
 DEGREES OF FREEDOM 3
POLY:Hit RETURN to continue
POLY: @@ There is an error if MgSiO3 is used instead of the
POLY: @@ defined Si1Mg1O3, since MgSiO3 is not defined as
POLY: @@ a species.
POLY:
POLY: s-c t=2200,p=2e10
   ... the command in full is SET_CONDITION
POLY: save tcex20 y
   ... the command in full is SAVE_WORKSPACES
POLY: @@ There is no degree of freedom with respect
POLY: @@ to oxygen so set its activity to unity (or
POLY: @@ any positive number)
POLY:
POLY: s-c ac(o)=1
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
15:10:30,053 INFO  Preparing system for use: USER_1998433168_11_MODIFIED_15892026275169
15:10:34,297 INFO  Preparing phase for use: A_QUARTZ
15:10:34,452 INFO  Preparing phase for use: BETA_FORSTERITE
15:10:34,611 INFO  Preparing phase for use: B_QUARTZ
15:10:34,847 INFO  Preparing phase for use: CLINOENSTATITE
15:10:35,040 INFO  Preparing phase for use: CLINOENSTHP
15:10:35,259 INFO  Preparing phase for use: COESITE
15:10:35,492 INFO  Preparing phase for use: CRISTOBALITE
15:10:35,612 INFO  Preparing phase for use: FORSTERITE
15:10:35,738 INFO  Preparing phase for use: GAMMA_FORSTERITE
15:10:35,874 INFO  Preparing phase for use: GARNET_MG
15:10:35,981 INFO  Preparing phase for use: ILMENITE_MG
15:10:36,121 INFO  Preparing phase for use: MG_PEROVSKITE
15:10:36,227 INFO  Preparing phase for use: ORTHOENSTATITE
15:10:36,325 INFO  Preparing phase for use: PERICLASE
15:10:36,456 INFO  Preparing phase for use: STISHOVITE
15:10:36,645 INFO  Preparing phase for use: TRIDYMITE
 Testing POLY result by global minimization procedure
Calculated            16 grid points in             0 s
    31 ITS,  CPU TIME USED  11 SECONDS
POLY: save tcex20 y
   ... the command in full is SAVE_WORKSPACES
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 GARNET_MG               ENTERED      0.000000E+00    4.000000E+01
 BETA_FORSTERITE         ENTERED      0.000000E+00    2.400000E+02
 GAMMA_FORSTERITE        ENTERED     -5.946730E-03    0.000000E+00
 MG_PEROVSKITE           ENTERED     -2.558352E-02    0.000000E+00
 ILMENITE_MG             ENTERED     -4.828445E-02    0.000000E+00
 PERICLASE               ENTERED     -9.575143E-02    0.000000E+00
 CLINOENSTHP             ENTERED     -1.541632E-01    0.000000E+00
 ORTHOENSTATITE          ENTERED     -2.197450E-01    0.000000E+00
 CLINOENSTATITE          ENTERED     -2.394369E-01    0.000000E+00
 FORSTERITE              ENTERED     -2.417190E-01    0.000000E+00
 STISHOVITE              ENTERED     -3.053984E-01    0.000000E+00
 COESITE                 ENTERED     -3.775316E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -7.835592E+00
 A_QUARTZ B_QUARTZ TRIDYMITE CRISTOBALITE
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: X
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 N(MGO)=180, N(SIO2)=100, T=2200, P=2E10, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature   2200.00 K (  1926.85 C),  Pressure  2.000000E+10
 Number of moles of components  2.80000E+02,  Mass in grams  1.32632E+04
 Total Gibbs energy -1.80863E+08,  Enthalpy -9.91578E+07,  Volume  3.55512E-03

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 MGO                     1.8000E+02  6.4286E-01 7.6674E-14 -5.5240E+05 SER
 O                       0.0000E+00  0.0000E+00 1.0000E+00  0.0000E+00 SER
 SIO2                    1.0000E+02  3.5714E-01 4.6393E-20 -8.1430E+05 SER

 BETA_FORSTERITE             Status ENTERED     Driving force  0.0000E+00
 Moles 2.4000E+02, Mass 1.1255E+04, Volume fraction 8.5320E-01  Mole fractions:
 MGO   6.66667E-01  SIO2  3.33333E-01  O     0.00000E+00

 GARNET_MG                   Status ENTERED     Driving force  0.0000E+00
 Moles 4.0000E+01, Mass 2.0078E+03, Volume fraction 1.4680E-01  Mole fractions:
 MGO   5.00000E-01  SIO2  5.00000E-01  O     0.00000E+00
POLY:Hit RETURN to continue
POLY:
POLY: ent fun dens=1e-3*bm/vm;
   ... the command in full is ENTER_SYMBOL
POLY: sh dens
   ... the command in full is SHOW_VALUE
 DENS=3730.7358
POLY: @@ We have found the equilibrium at this pressue.
POLY: @@ Now assume this system is decompressed
POLY: @@ adiabatically. What will the new temperature become?
```

```
POLY:
POLY: s-c h
   ... the command in full is SET_CONDITION
Value /-99157833.21/:
POLY: s-c t
   ... the command in full is SET_CONDITION
Value /2200/: none
POLY: 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:Hit RETURN to continue
POLY: @@ Now t is independent, calculate the equilibrium and get t
POLY:
POLY: 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: sh t
   ... the command in full is SHOW_VALUE
 T=2200.
POLY:Hit RETURN to continue
POLY: @@ It's the same temperature. Now change pressure
POLY:
POLY: s-c p
   ... the command in full is SET_CONDITION
Value /2E+10/: 150e8
POLY: 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: sh t
   ... the command in full is SHOW_VALUE
 T=2977.6276
POLY:Hit RETURN to continue
POLY: @@ We will also have a new density and another set of
POLY: @@ stable phases.
POLY:
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 N(MGO)=180, N(SIO2)=100, P=1.5E10, AC(O)=1, H=-9.91578E7
 DEGREES OF FREEDOM 0

 Temperature   2977.63 K (  2704.48 C),  Pressure  1.500000E+10
 Number of moles of components  2.80000E+02,  Mass in grams  1.32632E+04
 Total Gibbs energy -2.30661E+08,  Enthalpy -9.91578E+07,  Volume  3.59115E-03

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 MGO                     1.8000E+02  6.4286E-01 4.6875E-13 -7.0283E+05 SER
 O                       0.0000E+00  0.0000E+00 1.0000E+00  0.0000E+00 SER
 SIO2                    1.0000E+02  3.5714E-01 5.3688E-19 -1.0415E+06 SER

 GARNET_MG                   Status ENTERED     Driving force  0.0000E+00
 Moles 2.0000E+02, Mass 1.0039E+04, Volume fraction 7.4847E-01  Mole fractions:
 MGO   5.00000E-01  SIO2  5.00000E-01  O     0.00000E+00

 PERICLASE                   Status ENTERED     Driving force  0.0000E+00
 Moles 8.0000E+01, Mass 3.2244E+03, Volume fraction 2.5153E-01  Mole fractions:
 MGO   1.00000E+00  SIO2  0.00000E+00  O     0.00000E+00
POLY: sh dens
   ... the command in full is SHOW_VALUE
 DENS=3693.3029
POLY: sh v
   ... the command in full is SHOW_VALUE
 V=3.5911547E-3
POLY: sh vm
   ... the command in full is SHOW_VALUE
 VM=1.2825553E-5
POLY:
POLY: set-inter
   ... the command in full is SET_INTERACTIVE
POLY:
```

tcex21

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex21\tcex21.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a ternary isotherm in Fe-Cr-Ni
SYS:
SYS: @@ This example calculates a ternary isotherm
SYS: @@ in Fe-Cr-Ni with a user-defined database.
SYS:
SYS: set-log ex21,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: 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
15:11:53,731 INFO  USER_1113142095_11, number of lines read: 195
15:11:54,183 INFO  Parsing of USER_1113142095_11 completed in 553 ms
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
15:11:54,338 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A.T. Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4, p 317-425; '
  'J.O. Andersson, B. Sundman, Calphad 11(1987)1 p 83-92 TRITA-MAC 270
      (1986); Cr-Fe'
  'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
  'Byeong-Joo Lee, Calphad 16(1992)2, p 121-149; carbides'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Fe-Ni'
  'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Cr-Ni'
  'A.F. Guillermet, Z. Metallkde. 79(1988)8 p 524-536, TRITA-MAC 362 (1988);
      C-Co-Ni, C-Co-Fe-Ni'
  'K. Frisk, Metall. Trans. 21A (1990)9 p 2477-2488, Cr-Fe-N'
  'Unassessed parameter, linear combination of unary data.'
  'P. Gustafson, Calphad 12(1987)3 p 277-292, Cr-Ni-W '
 -OK-
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ With 3 components we must set 5 conditions

POLY: s-c t=1073 p=1e5 n=1 x(cr)=.2 x(ni)=.2
   ... the command in full is SET_CONDITION
POLY: 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:
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
15:11:55,266 INFO  Preparing system for use: USER_1113142095_11
15:11:56,152 INFO  Preparing phase for use: LIQUID
15:11:56,513 INFO  Preparing phase for use: BCC_A2
15:11:56,666 INFO  Preparing phase for use: FCC_A1
15:11:56,815 INFO  Preparing phase for use: HCP_A3
15:11:56,977 INFO  Preparing phase for use: SIGMA
Calculated          9684 grid points in             4 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     4  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1073, P=1E5, N=1, X(CR)=0.2, X(NI)=0.2
```

```
 DEGREES OF FREEDOM 0

 Temperature   1073.00 K (   799.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.56454E+01
 Total Gibbs energy -5.39559E+04,  Enthalpy  3.01555E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                      2.0000E-01  1.8688E-01 5.8626E-03 -4.5849E+04 SER
 FE                      6.0000E-01  6.0217E-01 3.1002E-03 -5.1533E+04 SER
 NI                      2.0000E-01  2.1094E-01 4.2164E-04 -6.9332E+04 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.5645E+01, Volume fraction 0.0000E+00  Mass fractions:
 FE  6.02174E-01  NI  2.10943E-01  CR  1.86883E-01
POLY:Hit RETURN to continue
POLY: @@ Define axis
POLY: s-a-v 1 x(cr) 0 1,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 x(ni) 0 1,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex21 y
   ... the command in full is SAVE_WORKSPACES
POLY: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 ERROR                   1611 when calculating equilibrium
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18

 Phase region boundary   1 at:   3.521E-02  1.510E-02
     BCC_A2
  ** FCC_A1
 Calculated.                      20 equilibria

 Phase region boundary   2 at:   2.615E-01  6.190E-02
     BCC_A2
  ** FCC_A1
  ** SIGMA

 Phase region boundary   3 at:   3.723E-01  3.566E-02
     BCC_A2
  ** SIGMA
 Calculated                      21 equilibria

 Phase region boundary   4 at:   3.168E-01  6.107E-02
     FCC_A1
  ** SIGMA
 Calculated.                      20 equilibria

 Phase region boundary   5 at:   4.140E-01  2.295E-01
  ** BCC_A2
     FCC_A1
  ** SIGMA

 Phase region boundary   6 at:   5.304E-01  1.820E-01
  ** BCC_A2
     FCC_A1
 Calculated                      43 equilibria

 Phase region boundary   7 at:   6.616E-01  7.178E-02
  ** BCC_A2
     SIGMA
 Calculated                      31 equilibria

 Phase region boundary   8 at:   2.615E-01  6.190E-02
     BCC_A2
  ** FCC_A1
 Calculated                      33 equilibria

 Phase region boundary   9 at:   3.521E-02  1.510E-02
     BCC_A2
  ** FCC_A1
 Calculated                      15 equilibria

 Phase region boundary  10 at:   1.095E-02  2.044E-02
     BCC_A2
  ** FCC_A1
 Calculated                      18 equilibria

 Phase region boundary  11 at:   1.095E-02  2.044E-02
     BCC_A2
  ** FCC_A1
 Calculated.                      22 equilibria
 Terminating at known equilibrium

 Phase region boundary  12 at:   3.838E-01  1.780E-02
```

```
    BCC_A2
 ** SIGMA
 Calculated.                      2 equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   3.838E-01  1.780E-02
    BCC_A2
 ** SIGMA
 Calculated                     21 equilibria

 Phase region boundary  14 at:   5.848E-01  2.838E-02
    BCC_A2
 ** SIGMA
 Calculated                     32 equilibria

 Phase region boundary  15 at:   5.848E-01  2.838E-02
    BCC_A2
 ** SIGMA
 Calculated.                      8 equilibria
 Terminating at known equilibrium

 Phase region boundary  16 at:   5.404E-01  9.033E-03
    BCC_A2
 ** SIGMA
 Calculated                     12 equilibria

 Phase region boundary  17 at:   5.404E-01  9.033E-03
    BCC_A2
 ** SIGMA
 Calculated.                     13 equilibria
 Terminating at known equilibrium

 Phase region boundary  18 at:   4.123E-01  2.273E-01
    FCC_A1
 ** SIGMA
 Calculated.                     19 equilibria
 Terminating at known equilibrium

 Phase region boundary  19 at:   4.123E-01  2.273E-01
    FCC_A1
 ** SIGMA
 Calculated.                      2 equilibria
 Terminating at known equilibrium

 Phase region boundary  20 at:   9.183E-03  2.090E-02
 ** BCC_A2
    FCC_A1
 Calculated                     13 equilibria

 Phase region boundary  21 at:   9.183E-03  2.090E-02
 ** BCC_A2
    FCC_A1
 Calculated.                     22 equilibria
 Terminating at known equilibrium

 Phase region boundary  22 at:   6.363E-01  2.710E-01
 ** BCC_A2
    FCC_A1
 Calculated.                     16 equilibria
 Terminating at known equilibrium

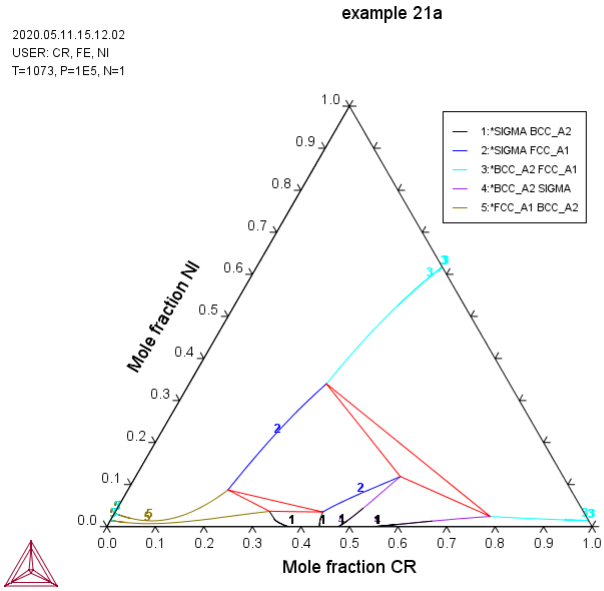
 Phase region boundary  23 at:   6.363E-01  2.710E-01
 ** BCC_A2
    FCC_A1
 Calculated                     26 equilibria

 Phase region boundary  24 at:   6.789E-01  3.114E-01
 ** BCC_A2
    FCC_A1
 Calculated.                     22 equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   6.789E-01  3.114E-01
 ** BCC_A2
    FCC_A1
 Calculated                     16 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex21\tcex21.POLY3
 CPU time for mapping                     4 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST: set-title example 21a
POST: se-d-ty y,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-l b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex22

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex22\tcex22.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating an adiabatic flame temperature
SYS:
SYS: @@ This example examines a heat balance when C3H8 is burned
SYS: @@ in oxygen by calculating the adiabatic flame temperature.
SYS: @@ Note that a SSUB database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex22,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw ssub6
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v6.0

 VA  DEFINED
TDB_SSUB6: def-sys c o h
   ... the command in full is DEFINE_SYSTEM
 C                       O                       H
   DEFINED
TDB_SSUB6: get
   ... the command in full is GET_DATA
15:13:27,055 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
      C1<G> C<G>
   C1H1<G> T.C.R.A.S. Class: 2
      C1H1<G> CH<G>
   C1H1O1<G> T.C.R.A.S. Class: 4
      C1H1O1<G> HCO<G>
      FORMYL <GAS>
   C1H1O2<G> T.C.R.A.S. Class: 6
      C1H1O2<G>
   C1H2<G> T.C.R.A.S. Class: 5
      METHYLENE
      METHYLENE <GAS>
   C1H2O1<G> T.C.R.A.S. Class: 5
      C1H2O1<G> CH2O<G>
      FORMALDEHYDE <GAS>
   C1H2O2_CIS<G> T.C.R.A.S. Class: 5
      C1H2O2_CIS<G>
   C1H2O2_DIOXIRANE<G> T.C.R.A.S. Class: 6
      C1H2O2_DIOXIRANE<G>
      S298 corrected and cp refitted
      due to corrected data in IVTAN2000 7/2002
   C1H2O2_TRANS<G> T.C.R.A.S. Class: 5
      C1H2O2_TRANS<G>
   C1H3<G> T.C.R.A.S. Class: 5
      METHYL Gaseous Standard State.
      METHYL <GAS>
   C1H3O1_CH2OH<G> T.C.R.A.S. Class: 6
      C1H3O1_CH2OH<G>
   C1H3O1_CH3O<G> T.C.R.A.S. Class: 5
      C1H3O1_CH3O<G>
   C1H4<G> T.C.R.A.S. Class: 5
      METHANE. Gaseous Standard State.
      METHANE <GAS>
   C1H4O1<G> T.C.R.A.S. Class: 5
      C1H4O1<G> CH3OH<G>
      METHANOL <GAS>
   C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      C1O1<G> CO<G>
      CARBON MONOXIDE <GAS>
      STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
   C1O2<G> T.C.R.A.S. Class: 2
      C1O2<G> CO2<G>
      CARBON DIOXIDE <GAS>
   C2<G> T.C.R.A.S. Class: 2
      CARBON Diatomic Gas.
      CARBON <DIATOMIC GAS>
   C2H1<G> T.C.R.A.S. Class: 6
      C2H1<G> C2H<G>
      CCH RADICAL <GAS>
   C2H2<G> T.C.R.A.S. Class: 2
      ACETYLENE (ETYNE). Gaseous Standard State.
      ACETYLENE <GAS>
   C2H2O1<G> T.C.R.A.S. Class: 6
      C2H2O1<G>
      OXIRENE
      S298 corrected and cp refitted
      due to corrected data in IVTAN2000 7/2002
   C2H3<G> T.C.R.A.S. Class: 6
```

DICARBON TRIHYDRIDE Gaseous Standard State.
C2H4<G> T.C.R.A.S. Class: 6
ETHYLENE. Gaseous Standard State.
ETHYLENE <GAS>
C2H4O1_ACETALDEHYDE<G> T.C.R.A.S. Class: 5
C2H4O1_ACETALDEHYDE<G>
C2H4O1_OXIRANE<G> T.C.R.A.S. Class: 6
C2H4O1_OXIRANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C2H4O2_ACETICACID<G> T.C.R.A.S. Class: 5
C2H4O2_ACETICACID<G>
C2H4O2_DIOXETANE<G> T.C.R.A.S. Class: 6
C2H4O2_DIOXETANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
typing error corrected 12/06
C2H4O3_123TRIOXOLANE<G> T.C.R.A.S. Class: 7
C2H4O3_123TRIOXOLANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C2H4O3_124TRIOXOLANE<G> T.C.R.A.S. Class: 7
C2H4O3_124TRIOXOLANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
typing error corrected 12/06
C2H5<G> T.C.R.A.S. Class: 6
ETHYL radical. Gaseous Standard State.
C2H6<G> T.C.R.A.S. Class: 6
ETHANE. Gaseous Standard State.
C2H6O1_1<G> THERMODATA 04/98 TC
ETHANOL. Gaseous Standard State.
C2H6O1_2<G> THERMODATA 04/98 TC
DIMETHYL ETHER. Gaseous Standard State.
C2H6O2<G> THERMODATA
C2H6O2<G>
E-GLYCOL <GAS>.Data revised by THDA.
C2O1<G> T.C.R.A.S. Class: 5
C2O1<G>
C3<G> T.C.R.A.S. Class: 6
CARBON triatomic gas.
CARBON <TRIATOMIC GAS>
C3H1<G> T.C.R.A.S. Class: 6
C3H1<G>
2-PROPYNYLIDYNE
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C3H4_1<G> STULL WESTRUM SINKE 1969 SGTE
C3H4_1<G>
ALLENE = 1,2-PROPADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H4_2<G> STULL WESTRUM SINKE 1969 SGTE
C3H4_2<G>
PROPYNE (METHYLACETYLENE)
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H6O1_1<G> THERMODATA 04/98 TC
2-PROPENOL (ALLYL ALCOHOL). Gaseous Standard State.
C3H6O1_2<G> THERMODATA 04/98 TC
DL-METHYLOXIRANE. Gaseous Standard State.
C3H6_1<G> T.C.R.A.S. Class: 6 4.09.85
C3H6(G)Cyclopropane
C3H6_2<G> STULL WESTRUM SINKE 1969 SGTE
PROPENE
PROPENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H8<G> THERMODATA SGTE
PROPANE. Gaseous Standard State.
PROPANE <GAS>
PROPANE
C3O2<G> T.C.R.A.S. Class: 6
C3O2<G>
C4<G> T.C.R.A.S. Class: 7
C4<G>
C4H1<G> T.C.R.A.S Class: 6
1,3-BUTADIYNYL Gaseous Standard State.
1,3-BUTADIYNYL. Data provided by T.C.R.A.S. in 2000
C4H10_1<G> T.C.R.A.S Class: 4
BUTANE Gaseous Standard State.
BUTANE. Data provided by T.C.R.A.S. in 2000
C4H10_2<G> T.C.R.A.S Class: 4
METHYLPROPANE N-BUTANE Gaseous Standard State.
METHYLPROPANE N-BUTANE. Data provided by T.C.R.A.S. in 2000
C4H2_1<G> THERMODATA 1978 ST
1,3-BUTADIYNE. Gaseous Standard State.
C4H2_2<G> THERMODATA 06/93 ST
BUTADIYNE(BIACETYLENE). Gaseous Standard State.
C4H4_1<G> T.C.R.A.S Class: 6
1,3-CYCLOBUTADIENE Gaseous Standard State.
1,3-CYCLOBUTADIENE. Data provided by T.C.R.A.S. in 2000
C4H4_2<G> STULL WESTRUM SINKE 1969 SGTE
1-BUTEN-3-YNE VINYLACETYLENE. Gaseous Standard State.
1-BUTEN-3-YNE VINYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_1<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_1<G>
1,2-BUTADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_2<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_2<G>
1,3-BUTADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_3<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_3<G>
1-BUTYNE ETHYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_4<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_4<G>
2-BUTYNE DIMETHYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_5<G> T.C.R.A.S Class: 6
C4H6_5<G>
CYCLOBUTENE. Data provided by T.C.R.A.S. in 2000
C4H8_1<G> THERMODATA 04/98 TC
1-BUTENE. Gaseous Standard State.
C4H8_2<G> THERMODATA 04/98 TC
(E)-2-BUTENE. Gaseous Standard State.

C4H8_3<G> THERMODATA 04/98 TC
(Z)-2-BUTENE. Gaseous Standard State.
C4H8_4<G> THERMODATA 04/98 TC
CYCLOBUTANE. Gaseous Standard State.
C4H8_5<G> THERMODATA 04/98 TC
2-METHYLPROPENE. Gaseous Standard State.
C4H8_6<G> THERMODATA 04/98 TC
METHYLCYCLOPROPANE. Gaseous Standard State.
C5<G> T.C.R.A.S. Class: 7
C5<G>
C60<G> MHR-95
C60<G>
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the rotational
data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that
a frequency with degeneracy 5 is missing from list in [94Kor/Sid];
taken to be 419 cm-1, which gives very good, though not exact,
agreement with values quoted in [94Kor/Sid]. Note discrepancy
between calculated DrS(298) = -8943.5 J mol K-1 for the reaction
60C<g>=C60<g>and that given by [94Kor/Sid] in their Table 5,
-8950 J mol K-1. Enthalpy of formation: DfH = 2588 kJ/mol from
DsubH(298.15K) = 166 +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure
values reproduced very well.
[91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).
C6H6<G> T.C.R.A.S Class: 5
BENZENE. Gaseous Standard State.
BENZENE. Data provided by T.C.R.A.S. in 2000
C6H6O1<G> THERMODATA 01/93
C6H6O1<G>
PHENOL
28/01/93
H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
H1<G> H<G>
HYDROGEN <MONATOMIC GAS>
H1O1<G> T.C.R.A.S. Class: 1
H1O1<G> OH<G>
H1O2<G> T.C.R.A.S. Class: 4
H1O2<G>
H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
H2<G> H2<G>
HYDROGEN<G>
STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
H2O1<G> T.C.R.A.S. Class: 1
H2O1<G> H2O<G>
WATER <GAS>
H2O2<G> JANAF SECOND EDIT SGTE
H2O2<G> H2O2<G>
HYDROGEN PEROXIDE <GAS>
O1<G> TCRAS 02/06/80
O1 Gaseous Standard State.
O2<G> TCRAS 21/06/90
OXYGEN Gaseous Standard State.
O3<G> TCRAS 02/06/80
OZONE Gaseous Standard State.
C1H2O2<L> THERMODATA 01/93
C1H2O2 HCOOH
FORMIC ACID MONOMERIC
28/01/93
C1H4O1<L> I. BARIN 3rd. Edition
C1H4O1 CH3OH
METHANOL. H298 and S298 modified.
C1H4<L> THERMODATA 04/99 HH
METHANE Liquid Standard State.
C2H4O2<L> THERMODATA 01/93
C2H4O2
ACETIC ACID
28/01/93 Tb=389K.
C2H6O1<L> THERMODATA 01/93
C2H6O1 C2H6O
ETHANOL
28/01/93
C2H6O2<L> THERMODATA
C2H6O2
E-GLYCOL
Data revised by THDA.
C2H6<L> THERMODATA 04/99 HH
ETHANE Liquid Standard State.
C3H6<L> THERMODATA 03/05 HH
CYCLOPROPANE. Liquid Standard State.
C3H8<L> THERMODATA 04/99 HH
PROPANE Liquid Standard State
C4H8<L> THERMODATA 04/99 HH
CYCLOBUTANE. Liquid Standard State.
C60 MHR-95
C60
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.
The
Fitted to the data in [94Kor/Sid], who took the phase transition at
257K
that [94Kor/Sid] do not give an explicit value for S(298.15K).
S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =425.8 and Cp
e
calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]
in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.
Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
the value preferred, if obliquely, by [94Kor/Sid].
[92Ste/Chi]W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,
P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).
C6H6<L> THERMODATA 04/99 BC
BENZENE. Liquid Standard State. Tm=278.6K
C1 S.G.T.E. **
GRAPHITE
Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
C1<DIAMOND> S.G.T.E. **
C1<DIAMOND> <DIAMOND>
DIAMOND
Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
from 1994 database (ex THERMODATA 01/93)
H2O1<L> T.C.R.A.S. Class: 4
H2O1 H2O
WATER
T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002
H2O2<L> THERMODATA 01/93
H2O2 H2O2
HYDROGEN PEROXIDE
28/01/93

```
 -OK-
TDB_SSUB6: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 C                        ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 H2O2_L                   ENTERED      0.000000E+00    0.000000E+00
 H2O1_L                   ENTERED      0.000000E+00    0.000000E+00
 DIAMOND                  ENTERED      0.000000E+00    0.000000E+00
 C_S                      ENTERED      0.000000E+00    0.000000E+00
 C_L                      ENTERED      0.000000E+00    0.000000E+00
 C6H6_L                   ENTERED      0.000000E+00    0.000000E+00
 C60_S                    ENTERED      0.000000E+00    0.000000E+00
 C4H8_L                   ENTERED      0.000000E+00    0.000000E+00
 C3H8_L                   ENTERED      0.000000E+00    0.000000E+00
 C3H6_L                   ENTERED      0.000000E+00    0.000000E+00
 C2H6_L                   ENTERED      0.000000E+00    0.000000E+00
 C2H6O2_L                 ENTERED      0.000000E+00    0.000000E+00
 C2H6O1_L                 ENTERED      0.000000E+00    0.000000E+00
 C2H4O2_L                 ENTERED      0.000000E+00    0.000000E+00
 C1H4_L                   ENTERED      0.000000E+00    0.000000E+00
 C1H4O1_L                 ENTERED      0.000000E+00    0.000000E+00
 C1H2O2_L                 ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 C                     ENTERED    C3H6                  ENTERED
 C1H1                  ENTERED    C3H6O1_1              ENTERED
 C1H1O1                ENTERED    C3H6O1_2              ENTERED
 C1H1O2                ENTERED    C3H6_1                ENTERED
 C1H2                  ENTERED    C3H6_2                ENTERED
 C1H2O1                ENTERED    C3H8                  ENTERED
 C1H2O2                ENTERED    C3O2                  ENTERED
 C1H2O2_CIS            ENTERED    C4                    ENTERED
 C1H2O2_DIOXIRANE      ENTERED    C4H1                  ENTERED
 C1H2O2_TRANS          ENTERED    C4H10_1               ENTERED
 C1H3                  ENTERED    C4H10_2               ENTERED
 C1H3O1_CH2OH          ENTERED    C4H2_1                ENTERED
 C1H3O1_CH3O           ENTERED    C4H2_2                ENTERED
 C1H4                  ENTERED    C4H4_1                ENTERED
 C1H4O1                ENTERED    C4H4_2                ENTERED
 C1O1                  ENTERED    C4H6_1                ENTERED
 C1O2                  ENTERED    C4H6_2                ENTERED
 C2                    ENTERED    C4H6_3                ENTERED
 C2H1                  ENTERED    C4H6_4                ENTERED
 C2H2                  ENTERED    C4H6_5                ENTERED
 C2H2O1                ENTERED    C4H8                  ENTERED
 C2H3                  ENTERED    C4H8_1                ENTERED
 C2H4                  ENTERED    C4H8_2                ENTERED
 C2H4O1_ACETALDEHYDE   ENTERED    C4H8_3                ENTERED
 C2H4O1_OXIRANE        ENTERED    C4H8_4                ENTERED
 C2H4O2                ENTERED    C4H8_5                ENTERED
 C2H4O2_ACETICACID     ENTERED    C4H8_6                ENTERED
 C2H4O2_DIOXETANE      ENTERED    C5                    ENTERED
 C2H4O3_123TRIOXOLANE ENTERED    C60                   ENTERED
 C2H4O3_124TRIOXOLANE ENTERED    C6H6                  ENTERED
 C2H5                  ENTERED    C6H6O1                ENTERED
 C2H6                  ENTERED    H                     ENTERED
 C2H6O1                ENTERED    H1O1                  ENTERED
 C2H6O1_1              ENTERED    H1O2                  ENTERED
 C2H6O1_2              ENTERED    H2                    ENTERED
 C2H6O2                ENTERED    H2O1                  ENTERED
 C2O1                  ENTERED    H2O2                  ENTERED
 C3                    ENTERED    O                     ENTERED
 C3H1                  ENTERED    O2                    ENTERED
 C3H4_1                ENTERED    O3                    ENTERED
 C3H4_2                ENTERED    VA                    ENTERED
POLY: @@ We need to know the heat content of C3H8<G> at room

POLY: @@ temperature. This is a simple number to look up in a
POLY: @@ table but actually quite tricky to calculate as pure
POLY: @@ C3H8 at room temperature does not represent an
POLY: @@ equilibrium state. However, you can get it as follows.
POLY:
POLY: s-c t=298.15,p=1e5,n(o)=1e-10
   ... the command in full is SET_CONDITION
POLY: s-i-a n(c3h8)=1
   ... the command in full is SET_INPUT_AMOUNTS
POLY: c-s p *=sus
   ... the command in full is CHANGE_STATUS
POLY: c-s p gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/:
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated            76 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: @@ The equilibrium state at room temperature is listed
POLY: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB6

 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  C1H2O1        4.96084E-27  C4H6_3        1.00000E-30
 C6O           8.16678E-03  C1H2O2_CIS    4.88436E-27  C2H4O1_OXIRA  1.00000E-30
 C6H6          1.38456E-03  C4H6_4        3.94602E-28  C4H6_5        1.00000E-30
 C2H6          1.00313E-04  C3H4_2        6.04110E-29  C5            1.00000E-30
 C3H8          5.44582E-07  C2H5          1.32230E-29  C2H3          1.00000E-30
 C4H10_2       3.84975E-08  C1H2O2_TRANS  6.61825E-30  C2H2O1        1.00000E-30
 H2            7.83769E-09  C3H4_1        2.45341E-30  C2H2          1.00000E-30
 C4H10_1       6.16323E-09  C4H6_1        2.07866E-30  C2H1          1.00000E-30
 C1O2          2.32090E-11  C             1.00000E-30  C2            1.00000E-30
 H2O1          2.50979E-12  C3O2          1.00000E-30  H             1.00000E-30
 C1O1          7.01016E-13  C4            1.00000E-30  H1O1          1.00000E-30
 C4H8_5        6.29486E-14  C3H6O1_2      1.00000E-30  H1O2          1.00000E-30
 C3H6_2        5.52670E-14  C3H6O1_1      1.00000E-30  H2O2          1.00000E-30
 C2H4          3.33175E-14  C4H1          1.00000E-30  C1H3O1_CH3O   1.00000E-30
 C4H8_2        7.83367E-15  C4H2_1        1.00000E-30  C1H3O1_CH2OH  1.00000E-30
 C4H8_3        3.33692E-15  C3H1          1.00000E-30  C1H3          1.00000E-30
 C4H8_1        4.53470E-16  C3            1.00000E-30  O             1.00000E-30
 C6H6O1        1.02341E-18  C2O1          1.00000E-30  C1H2O2_DIOXI  1.00000E-30
 C3H6_1        2.70389E-21  C2H6O2        1.00000E-30  O2            1.00000E-30
 C4H8_6        1.07592E-21  C2H6O1_2      1.00000E-30  O3            1.00000E-30
 C4H6_2        4.91032E-22  C4H2_2        1.00000E-30  C1H2          1.00000E-30
 C2H4O1_ACETA  1.25014E-22  C4H4_1        1.00000E-30  C1H1O2        1.00000E-30
 C4H8_4        2.10624E-23  C4H4_2        1.00000E-30  C1H1O1        1.00000E-30
 C2H4O2_ACETI  9.64309E-24  C2H4O3_124TR  1.00000E-30  C1H1          1.00000E-30
 C2H6O1_1      1.76369E-24  C2H4O3_123TR  1.00000E-30
 C1H4O1        1.08754E-24  C2H4O2_DIOXE  1.00000E-30
POLY: @@ The enthalpy for the system is
POLY: sh h
   ... the command in full is SHOW_VALUE
 H=-106064.27
POLY:Hit RETURN to continue
POLY: @@ But we want a gas with just C3H8.
POLY: @@ Use the Set-All-Startvalues command.
POLY: 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: sh h
   ... the command in full is SHOW_VALUE
 H=-99431.45
POLY: @@ The difference in H for the two calculations is actually
POLY: @@ not very large. The value is approximate but good as the
POLY: @@ enthalpy is calculated for the following gas constitution
POLY:
POLY: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB6

 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  1.07458E+01,  Mass in grams  4.32993E+01
 Total Gibbs energy -1.78580E+05,  Enthalpy -9.94314E+04,  Volume  2.43005E-02

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       2.9417E+00  8.1602E-01 1.1356E+07  4.0271E+04 SER
 H                       7.7974E+00  1.8150E-01 3.4211E-08 -4.2615E+04 SER
 O                       6.7105E-03  2.4795E-03 1.2651E-49 -2.7911E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 1.0746E+01, Mass 4.3299E+01, Volume fraction 1.0000E+00  Mass fractions:
 C  8.16017E-01  H  1.81504E-01  O  2.47953E-03
 Constitution:
 C3H8          9.70396E-01  C4H4_1        1.31579E-04  C2H4O2_ACETI  1.31579E-04
 C             1.31579E-04  C4H2_2        1.31579E-04  C2H4O1_OXIRA  1.31579E-04
 O2            1.31579E-04  C4H2_1        1.31579E-04  C2H4O1_ACETA  1.31579E-04
 O             1.31579E-04  C4H10_2       1.31579E-04  C2H4          1.31579E-04
 H2O2          1.31579E-04  C4H10_1       1.31579E-04  C2H3          1.31579E-04
 H2O1          1.31579E-04  C4H1          1.31579E-04  C2H2O1        1.31579E-04
 H2            1.31579E-04  C4            1.31579E-04  C2H2          1.31579E-04
 H1O2          1.31579E-04  C3O2          1.31579E-04  C2H1          1.31579E-04
 H1O1          1.31579E-04  O3            1.31579E-04  C2            1.31579E-04
 H             1.31579E-04  C3H6_2        1.31579E-04  C1O2          1.31579E-04
 C6H6O1        1.31579E-04  C3H6_1        1.31579E-04  C1O1          1.31579E-04
 C6H6          1.31579E-04  C3H6O1_2      1.31579E-04  C1H4O1        1.31579E-04
 C6O           1.31579E-04  C3H6O1_1      1.31579E-04  C1H4          1.31579E-04
 C5            1.31579E-04  C3H4_2        1.31579E-04  C1H3O1_CH3O   1.31579E-04
 C4H8_6        1.31579E-04  C3H4_1        1.31579E-04  C1H3O1_CH2OH  1.31579E-04
 C4H8_5        1.31579E-04  C3H1          1.31579E-04  C1H3          1.31579E-04
 C4H8_4        1.31579E-04  C3            1.31579E-04  C1H2O2_TRANS  1.31579E-04
 C4H8_3        1.31579E-04  C2O1          1.31579E-04  C1H2O2_DIOXI  1.31579E-04
 C4H8_2        1.31579E-04  C2H6O2        1.31579E-04  C1H2O2_CIS    1.31579E-04
 C4H8_1        1.31579E-04  C2H6O1_2      1.31579E-04  C1H2O1        1.31579E-04
 C4H6_5        1.31579E-04  C2H6O1_1      1.31579E-04  C1H2          1.31579E-04
 C4H6_4        1.31579E-04  C2H6          1.31579E-04  C1H1O2        1.31579E-04
 C4H6_3        1.31579E-04  C2H5          1.31579E-04  C1H1O1        1.31579E-04
 C4H6_2        1.31579E-04  C2H4O3_124TR  1.31579E-04  C1H1          1.31579E-04
 C4H6_1        1.31579E-04  C2H4O3_123TR  1.31579E-04
 C4H4_2        1.31579E-04  C2H4O2_DIOXE  1.31579E-04
POLY:Hit RETURN to continue
POLY: @@ We now have the initial amount of heat. Assuming an excess
POLY: @@ of oxygen we can calulate the temperature where the
POLY: @@ heat content would be the same
POLY:
POLY: sh h
   ... the command in full is SHOW_VALUE
 H=-99431.45
POLY: @@ H is just 11 times HM as there are 11 atoms in C3H8.
POLY: @@ Save that value in a variable
POLY:
POLY: enter var h298=h;
   ... the command in full is ENTER_SYMBOL
POLY: sh h298
   ... the command in full is SHOW_VALUE
 H298=-99431.45
```

```
POLY: @@ If all carbon and hydrogen react with oxygen we need 7
POLY: @@ oxygen atoms to form 3 moles C1O and 4 moles of H2O.
POLY: @@ Add some oxygen in excess
POLY:
POLY: s-c n(o)=9
   ... the command in full is SET_CONDITION
POLY: @@ Set the heat content as a condition and remove the
POLY: @@ condition on t
POLY:
POLY: s-c h=h298
   ... the command in full is SET_CONDITION
POLY: s-c t
   ... the command in full is SET_CONDITION
Value /298.15/: none
POLY: 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: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated            76 grid points in             0 s
   152 ITS,  CPU TIME USED   6 SECONDS
POLY: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB6

 Conditions:
 P=1E5, N(O)=9, N(C)=3, N(H)=8, H=H298
 DEGREES OF FREEDOM 0

 Temperature   3103.37 K (  2830.22 C),  Pressure  1.000000E+05
 Number of moles of components  2.00000E+01,  Mass in grams  1.88087E+02
 Total Gibbs energy -7.70691E+06,  Enthalpy -9.94314E+04,  Volume  2.20472E+00

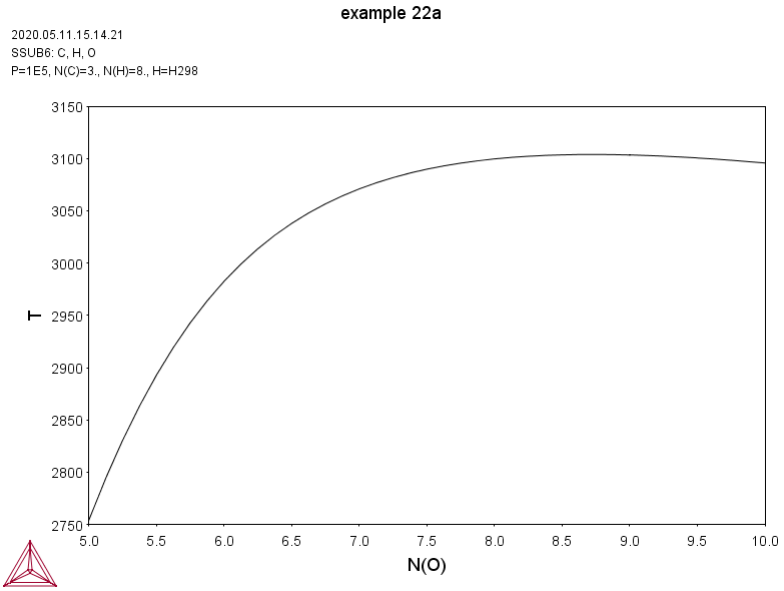
 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.0000E+00  1.9158E-01 9.3982E-09 -4.7691E+05 SER
 H                       8.0000E+00  4.2869E-02 7.7626E-06 -3.0360E+05 SER
 O                       9.0000E+00  7.6555E-01 6.3815E-08 -4.2748E+05 SER

 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          3.17918E-01  C1H2O2_DIOXI  7.89694E-16  C3H6O1_2      1.00000E-30
 C1O1          2.27799E-01  C2H1          8.90508E-17  C3H6_1        1.00000E-30
 C1O2          1.23305E-01  C3O2          8.73154E-17  C3H6_2        1.00000E-30
 H1O1          8.75243E-02  C2            1.57966E-17  C3H8          1.00000E-30
 H2            7.66545E-02  C2H2O1        2.52104E-18  C4            1.00000E-30
 O2            6.61854E-02  C2H3          2.72613E-19  C4H1          1.00000E-30
 H             5.95645E-02  C2H4O1_ACETA  1.22421E-20  C4H10_1       1.00000E-30
 O             4.10043E-02  C2H4          1.12666E-20  C4H10_2       1.00000E-30
 H1O2          4.23460E-05  C2H4O2_ACETI  7.64173E-21  C4H4_1        1.00000E-30
 H2O2          1.60571E-06  C3H1          9.69741E-23  C4H8_4        1.00000E-30
 C1H1O1        9.35079E-07  C3            6.41061E-23  C4H8_5        1.00000E-30
 C1H1O2        6.80240E-07  C2H4O1_OXIRA  1.10545E-23  C4H4_2        1.00000E-30
 O3            3.00641E-08  C2H5          2.16426E-24  C4H6_1        1.00000E-30
 C1H2O2_CIS    1.60533E-08  C2H6          2.32872E-26  C4H6_2        1.00000E-30
 C1H2O2_TRANS  8.97486E-09  C2H6O1_1      6.05817E-27  C4H6_3        1.00000E-30
 C1H2O1        7.25807E-09  C2H6O2        8.46558E-28  C4H6_4        1.00000E-30
 C             5.41880E-11  C3H4_2        5.36473E-28  C4H8_6        1.00000E-30
 C1H1          5.71334E-12  C3H4_1        2.88191E-28  C4H6_5        1.00000E-30
 C1H2          2.82748E-12  C2H6O1_2      7.51593E-29  C5            1.00000E-30
 C1H3          2.09122E-12  C2H4O2_DIOXE  1.26866E-29  C60           1.00000E-30
 C2O1          1.16897E-12  C2H4O3_124TR  2.44145E-30  C4H8_1        1.00000E-30
 C1H3O1_CH2OH  8.94424E-13  C4H2_1        2.38485E-30  C6H6          1.00000E-30
 C1H4          1.80436E-13  C4H2_2        2.37831E-30  C6H6O1        1.00000E-30
 C1H3O1_CH3O   1.92548E-14  C4H8_3        1.00000E-30  C4H8_2        1.00000E-30
 C1H4O1        9.77820E-15  C2H4O3_123TR  1.00000E-30
 C2H2          1.14657E-15  C3H6O1_1      1.00000E-30
POLY: @@ The adiabatic temperature is
POLY: sh t
   ... the command in full is SHOW_VALUE
 T=3103.3658
POLY:Hit RETURN to continue
POLY: @@ Now calculate how the adiabatic temperature varies
POLY: @@ with the amount of oxygen
POLY:
POLY: s-a-v 1 n(o) 5 10
   ... the command in full is SET_AXIS_VARIABLE
Increment /.125/:
POLY: save tcex22 y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    9.00000
...OK

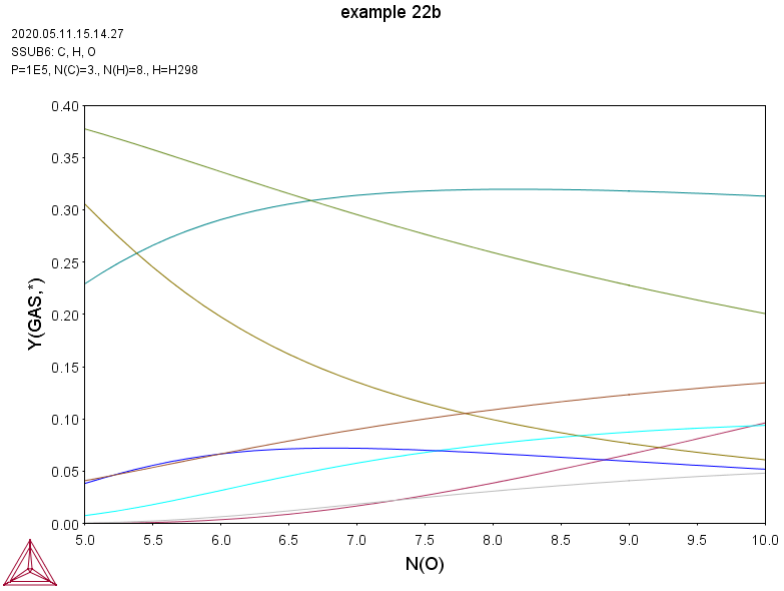
 Phase Region from    9.00000     for:
     GAS
 Global test at  1.00000E+01 .... OK
 Terminating at    10.0000
 Calculated    11 equilibria

 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: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex22\tcex22.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: s-d-a x n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22a
POST:
POST: SET_EXP_FILE_FORMAT 5
```

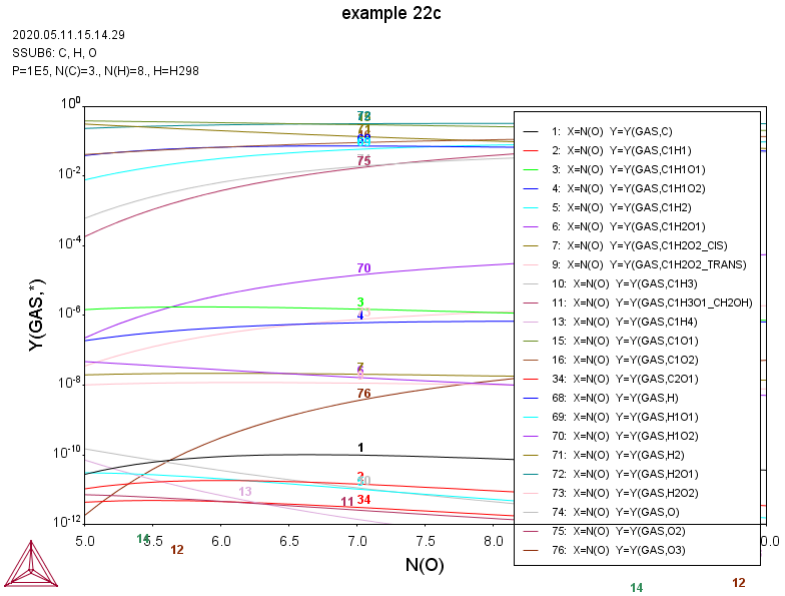
```
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



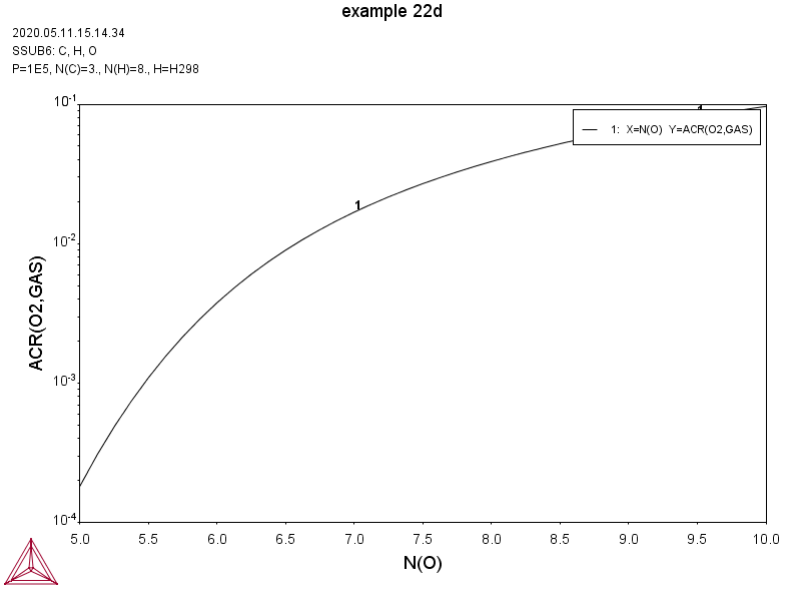

```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the gas constitition changes
POST: s-d-a y y(gas,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 22b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Add labels and a logarithmic fraction scale
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-s y n 1e-12 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 22c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

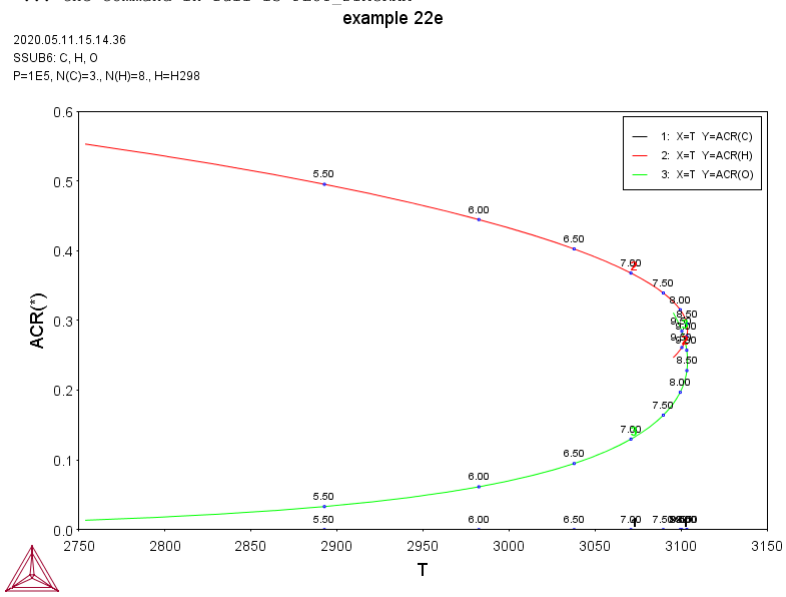



```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the oxygen partial pressure changes
POST: s-d-a y acr(o2,gas)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the activities of the components change
POST: @@ with temperature. Note that the oxygen content
POST: @@ also changes. Set the reference states
POST:
POST: set-ref-state o gas * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state h gas * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state c c_s * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: s-d-a x t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty y lin
   ... the command in full is SET_AXIS_TYPE
POST: s-d-a z n(o)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 5 10
   ... the command in full is SET_SCALING_STATUS
POST: s-d-a y acr(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 22e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
```

```
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex23

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex23\tcex23.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a paraequilibrium and the
SYS: @@ T0 temperature in a low alloyed steel
SYS:
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex23,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ Define the material

POLY: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: tcfe9
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: mn 1.5
2nd alloying element: si .3
Next alloying element: c .3
Next alloying element:
Temperature (C) /1000/: 700
 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
 REINITIATING GES .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 SI  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE                M23C6                    M7C3
 M5C2                     KSI_CARBIDE              FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14          M3SI
 MN9SI2                   MN11SI19                 MN6SI
 G_PHASE                  CR3SI                    FE2SI
 FESI2_H                  FESI2_L                  MSI
 M5SI3                    AL4C3                    FE8SI2C
 SIC                      MN5SIC                   CUZN_EPSILON
 AL5FE4                   MP_B31                   M2P_C22
 FLUORITE_C1:I            ZRO2_TETR:I              M2O3C:I
 M2O3H:I
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                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE                M23C6                    M7C3
 M5C2                     KSI_CARBIDE              FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14          M3SI
 MN9SI2                   MN11SI19                 MN6SI
 G_PHASE                  CR3SI                    FE2SI
 FESI2_H                  FESI2_L                  MSI
 M5SI3                    AL4C3                    FE8SI2C
 SIC                      MN5SIC                   CUZN_EPSILON
 AL5FE4                   MP_B31                   M2P_C22
 FLUORITE_C1:I            ZRO2_TETR:I              M2O3C:I
 M2O3H:I

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

OK? /Y/: Y
15:16:00,037 INFO  *** Invoking Gibbs Energy System v6 ***
 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
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C as it has net charge
Suspending M2O3H as it has net charge
Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE9
      database (TCFE v9.0, Jan, 2017).'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
  'I. Ansara, Unpublished work (1991); Cr-Si'
  'Unassessed parameter; Linear combination of unary data'
  'M. Seiersten, Unpublished work (1989); Al-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'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-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'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C
      and Al-Si-C'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
  'Thermo-Calc Software, Sweden, 2019: Volume data updated for TCFE9
      database (TCFE v9.1, June, 2019).'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
  'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6
      database (TCFE v6, April, 2008).'
  'NPL, Unpublished work (1989); C-Mn-Si'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
      and Fe-Mn-Nb'
  'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
      solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
      same phase as cubic Y2O3 (M2O3C).'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
      -21; Mn-Y-O'
  'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
      -64; Mn-Zr-O, Mn-Y-Zr-O'
  'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE8
      database (TCFE v8, May, 2015).'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid
      C-Fe-Si description'
  'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Fe-Nb-Si'
  'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
      Fe-P-Si'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         23501 grid points in             2 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     3  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -4.16107E+04,  Enthalpy  2.38957E+04,  Volume  7.24125E-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 6.6047E-03 -4.0618E+04 SER
 MN                       1.5035E-02  1.5000E-02 6.4366E-05 -7.8088E+04 SER
 SI                       5.8820E-03  3.0000E-03 2.0469E-10 -1.8051E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.3882E-01, Mass 4.1108E+01, Volume fraction 7.4531E-01  Mass fractions:
 FE  9.87913E-01  MN  8.77935E-03  SI  3.19719E-03  C   1.10618E-04

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 2.5520E-01, Mass 1.3887E+01, Volume fraction 2.5023E-01  Mass fractions:
```

```
 FE  9.57680E-01  MN  3.34923E-02  C   6.39607E-03  SI  2.43179E-03

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 5.9806E-03, Mass 7.1833E-02, Volume fraction 4.4546E-03  Mass fractions:
 C   1.00000E+00  SI  0.00000E+00  MN  0.00000E+00  FE  0.00000E+00
POLY: @@ Suspend some phases that normally never appear
POLY: ch-st p gra m5c2=sus
   ... the command in full is CHANGE_STATUS
POLY:Hit RETURN to continue
POLY: @@ Set axis for T-w(c) phase diagram
POLY: 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: 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: save tcex23a y
   ... the command in full is SAVE_WORKSPACES
POLY: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

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

 Phase region boundary   1 at:   2.500E-04  9.472E+02
     BCC_A2
     CEMENTITE
  ** FCC_A1
 Calculated.                      2 equilibria

 Phase region boundary   2 at:   6.590E-05  9.454E+02
     BCC_A2
  ** CEMENTITE
  ** FCC_A1

 Phase region boundary   3 at:   6.590E-05  9.454E+02
     BCC_A2
  ** FCC_A1
 Calculated                     16 equilibria

 Phase region boundary   4 at:   6.590E-05  9.454E+02
     BCC_A2
  ** CEMENTITE
 Calculated..                     11 equilibria
 Terminating at axis limit.

 Phase region boundary   5 at:   6.590E-05  9.454E+02
     BCC_A2
  ** CEMENTITE
     FCC_A1
 Calculated.                      31 equilibria

 Phase region boundary   6 at:   7.062E-03  9.920E+02
  ** BCC_A2
  ** CEMENTITE
     FCC_A1

 Phase region boundary   7 at:   7.062E-03  9.920E+02
  ** CEMENTITE
     FCC_A1
 Calculated..                     17 equilibria
 Terminating at axis limit.

 Phase region boundary   8 at:   7.062E-03  9.920E+02
  ** BCC_A2
     FCC_A1
 Calculated                     41 equilibria

 Phase region boundary   9 at:   7.062E-03  9.920E+02
  ** BCC_A2
```

```
    CEMENTITE
    FCC_A1
Calculated..                     13 equilibria
Terminating at axis limit.

Phase region boundary  10 at:   6.590E-05  9.454E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     42 equilibria
Terminating at axis limit.

Phase region boundary  11 at:   2.500E-04  9.472E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     41 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  12 at:   3.417E-03  9.670E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary  13 at:   3.417E-03  9.670E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  14 at:   6.583E-03  9.764E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     28 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   6.583E-03  9.764E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     16 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   5.334E-06  8.100E+02
    BCC_A2
 ** CEMENTITE
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  17 at:   5.334E-06  8.100E+02
    BCC_A2
 ** CEMENTITE
Calculated.                     10 equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   9.750E-03  9.821E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     40 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   9.750E-03  9.821E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                      3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   5.780E-05  9.367E+02
    BCC_A2
 ** CEMENTITE
Calculated..                     11 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  21 at:   5.780E-05  9.367E+02
    BCC_A2
 ** CEMENTITE
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   2.647E-03  1.063E+03
 ** BCC_A2
    FCC_A1
Calculated.                     19 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   2.647E-03  1.063E+03
 ** BCC_A2
    FCC_A1
Calculated                     22 equilibria

Phase region boundary  24 at:   8.894E-03  1.063E+03
 ** CEMENTITE
    FCC_A1
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   8.894E-03  1.063E+03
 ** CEMENTITE
    FCC_A1
Calculated..                      7 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  26 at:   2.500E-04  1.128E+03
```

```
  ** BCC_A2
     FCC_A1
 Calculated                      4 equilibria

 Phase region boundary  27 at:   2.500E-04  1.128E+03
  ** BCC_A2
     FCC_A1
 Calculated.                     29 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   3.417E-03  1.048E+03
  ** BCC_A2
     FCC_A1
 Calculated                     26 equilibria

 Phase region boundary  29 at:   3.417E-03  1.048E+03
  ** BCC_A2
     FCC_A1
 Calculated.                     16 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   6.583E-03  9.982E+02
  ** BCC_A2
     FCC_A1
 Calculated                     38 equilibria

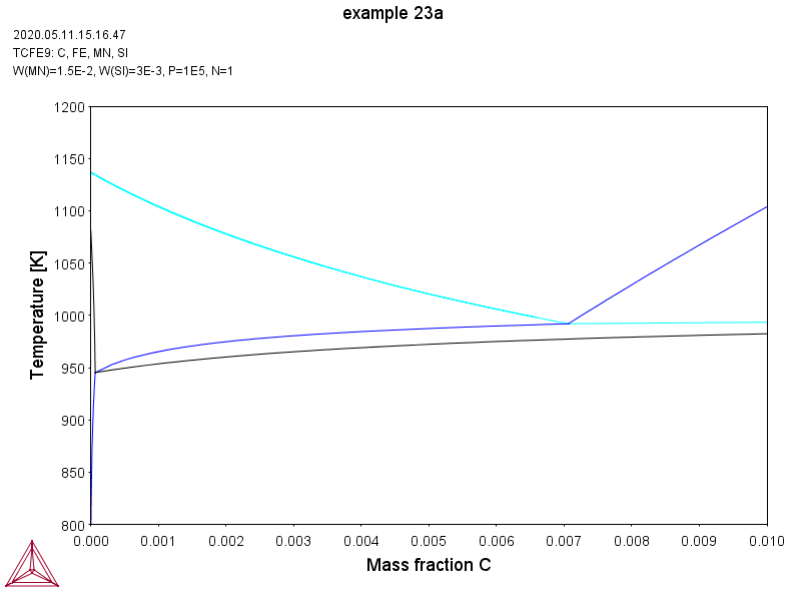
 Phase region boundary  31 at:   6.583E-03  9.982E+02
  ** BCC_A2
     FCC_A1
 Calculated.                      3 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   9.750E-03  1.095E+03
  ** CEMENTITE
     FCC_A1
 Calculated.                     12 equilibria
 Terminating at known equilibrium

 Phase region boundary  33 at:   9.750E-03  1.095E+03
  ** CEMENTITE
     FCC_A1
 Calculated..                      3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex23\tcex23a.POLY3
 CPU time for mapping                    13 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

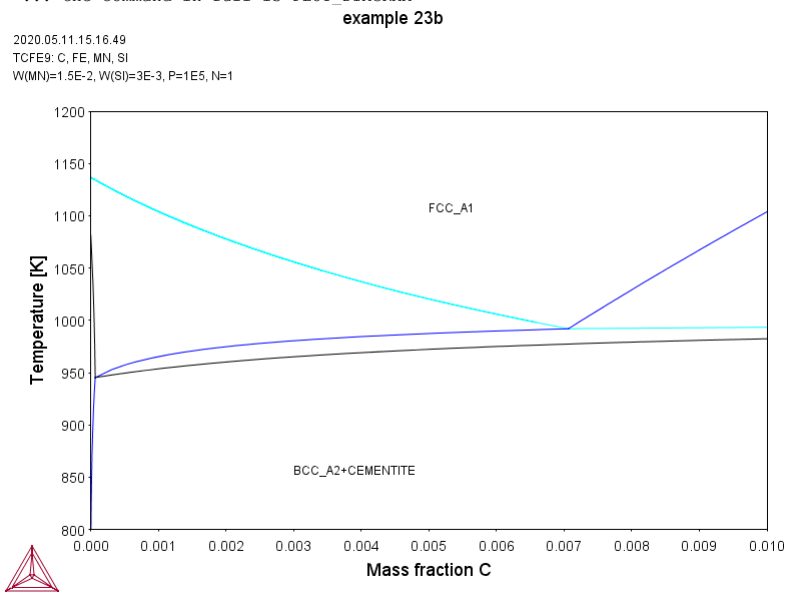
 Setting automatic diagram axes

POST:
POST: set-title example 23a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

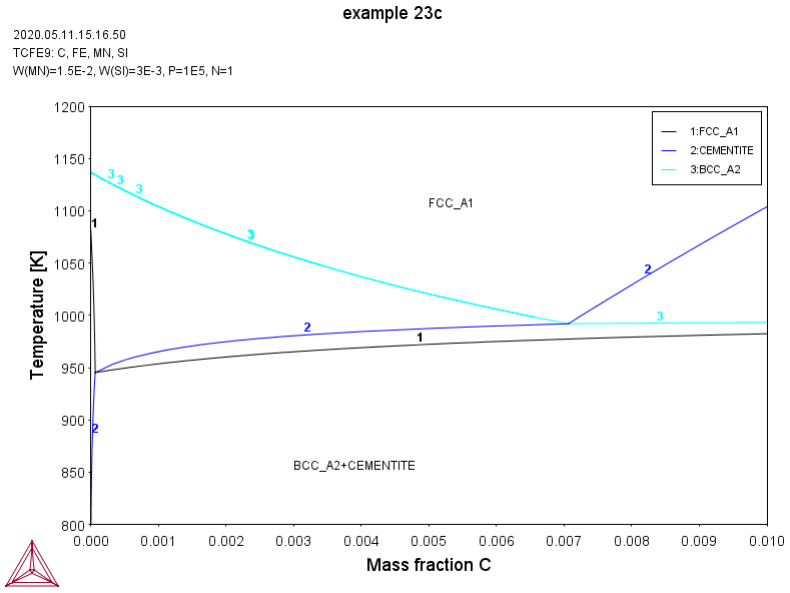



```
POST:
POST:Hit RETURN to continue
POST: @@ Add labels
POST: add
   ... the command in full is ADD_LABEL_TEXT
Give X coordinate in axis units: .005
Give Y coordinate in axis units: 1100
Automatic phase labels? /Y/: Y
 Automatic labelling not always possible
 Using global minimization procedure
Calculated         23291 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: FCC_A1
Text size: /.36/: .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         23291 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_A2+CEMENTITE
Text size: /.36/: .34
POST: set-title example 23b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-lab
   ... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: ?
 THE OPTIONS MEANS:
 A     LIST STABLE PHASES ALONG LINE
 B     AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
 C     LIST AXIS QUANTITIES
 D     AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
 E     AS B WITH CHANGING COLORS
 F     AS D WITH CHANGING COLORS
 N     NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: e
POST: set-title example 23c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY: @@ Now calculate the T-zero temperature for the steel
POLY: read tcex23a
   ... the command in full is READ_WORKSPACES
```

```
POLY: advanced-options
Which option? /STEP_AND_MAP/: ?
 EQUILIBRIUM_CALCUL       NEW_COMPOSITION_SET      STABILITY_CHECK
 GLOBAL_MINIMIZATION      OUTPUT_FILE_FOR_SHOW     STEP_AND_MAP
 IGNORE_COMPOSI_SET_ORDER PARAEQUILIBRIUM          T-ZERO TEMPERATURE
 KEEP_COMP_SET_NUMBERS    PHASE_ADDITION           TOGGLE_ALTERNATE_MODE
 LIST_PHASE_ADDITION      PRESENT_PHASE
 MAJOR_CONSTITUENTS       SHOW_FOR_T=
Which option? /STEP_AND_MAP/: t-z

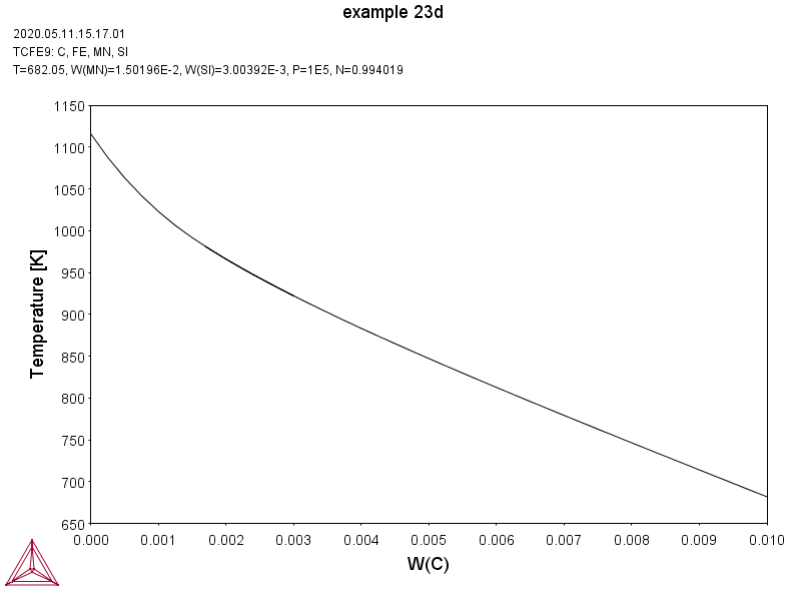
This command calculates the temperature when two phases have the same Gibbs
energy.  You must calculate an equilibrium at an estimated temperature first.
Name of first phase: fcc
Name of second phase: bcc

 The T0 temperature is  922.23 K
 Note: LIST-EQUILIBRIUM is not relevant
POLY:Hit RETURN to continue
POLY: @@ Calculate the T-zero line, remove the T-axis
POLY: 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: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex23b y
   ... the command in full is SAVE_WORKSPACES
POLY: 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         922.23
   2.750000E-03         932.57
   2.500000E-03         943.26
   2.250000E-03         954.39
   2.000000E-03         966.05
   1.750000E-03         978.40
   1.500000E-03         991.68
   1.250000E-03        1006.30
   1.000000E-03        1022.97
   7.500000E-04        1041.88
   5.000000E-04        1063.25
   2.500000E-04        1087.67
   2.500000E-10        1115.87

 Phase Region from   0.169775E-02 for:
     BCC_A2
     FCC_A1
   1.697751E-03         981.03
   1.947751E-03         968.51
   2.197751E-03         956.72
   2.447751E-03         945.49
   2.697751E-03         934.72
   2.947751E-03         924.31
   3.197751E-03         914.20
   3.447751E-03         904.36
   3.697751E-03         894.74
   3.947751E-03         885.31
   4.197751E-03         876.05
   4.447751E-03         866.93
   4.697751E-03         857.95
   4.947751E-03         849.08
   5.197751E-03         840.32
   5.447751E-03         831.64
   5.697751E-03         823.05
   5.947751E-03         814.53
   6.197751E-03         806.08
   6.447751E-03         797.69
   6.697751E-03         789.35
   6.947751E-03         781.05
   7.197751E-03         772.80
   7.447751E-03         764.59
   7.697751E-03         756.41
   7.947751E-03         748.26
   8.197751E-03         740.13
   8.447751E-03         732.03
   8.697751E-03         723.95
   8.947751E-03         715.88
   9.197751E-03         707.83
   9.447751E-03         699.79
   9.697751E-03         691.75
   9.947751E-03         683.73
   1.000000E-02         682.05
 *** Buffer savend on file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex23\TCEX23~2.POL
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: set-title example 23d
POST: s-d-a x w(c)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
```

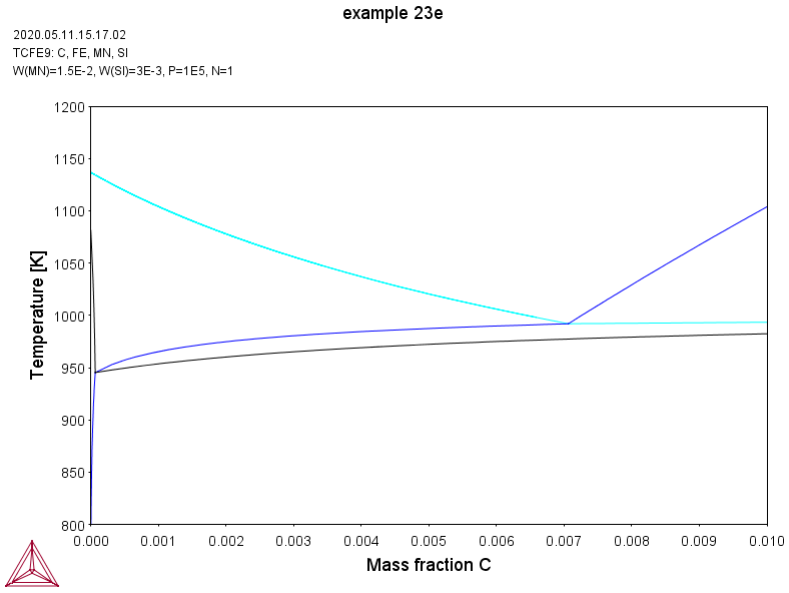
```
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



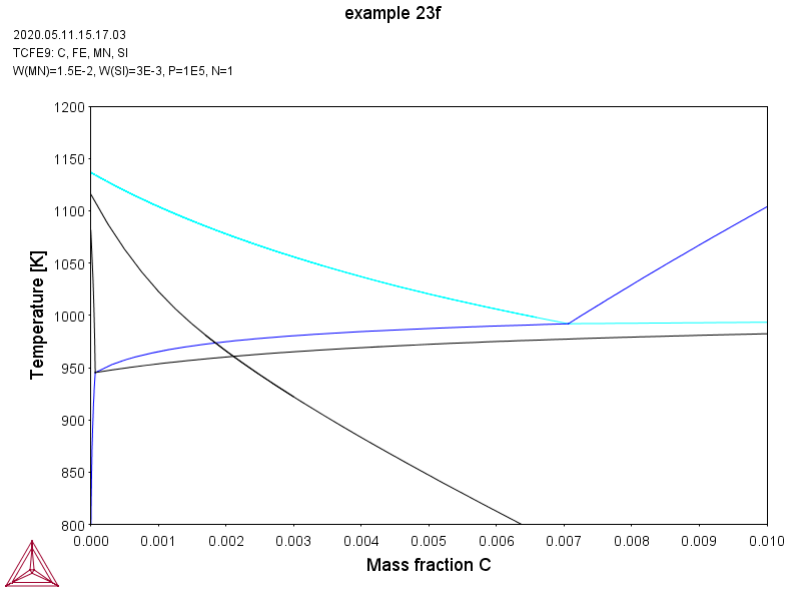

```
POST:
POST:Hit RETURN to continue
POST: @@ Write the line on a data file
POST: make tcex23b y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: ba
   ... the command in full is BACK
POLY: @@ Plot together with a phase diagram
POLY: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST: set-title example 23e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23b
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY: @@ Now calculate the paraequilibrium for the steel.
POLY: @@ At paraequilibrium only C is mobile, the other
POLY: @@ alloying elements have the same compositions in
POLY: @@ both phases
POLY:
POLY: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         23291 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: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -4.16100E+04,  Enthalpy  2.36447E+04,  Volume  7.22641E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        1.3754E-02  3.0000E-03 2.3004E-01 -1.1890E+04 SER
 FE                       9.6533E-01  9.7900E-01 6.6052E-03 -4.0617E+04 SER
 MN                       1.5035E-02  1.5000E-02 6.3295E-05 -7.8224E+04 SER
 SI                       5.8820E-03  3.0000E-03 2.0677E-10 -1.8043E+05 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.9478E-01, Mass 4.4221E+01, Volume fraction 8.0338E-01  Mass fractions:
 FE  9.88036E-01  MN  8.63188E-03  SI  3.22044E-03  C   1.12114E-04

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.7198E-01, Mass 9.3562E+00, Volume fraction 1.6894E-01  Mass fractions:
 FE  9.58088E-01  MN  3.30194E-02  C   6.45691E-03  SI  2.43593E-03

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 3.3247E-02, Mass 1.4901E+00, Volume fraction 2.7674E-02  Mass fractions:
 FE  8.42167E-01  MN  9.08384E-02  C   6.69948E-02  SI  4.69973E-13
POLY: 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) =   0.4278 with U-fractions C  =  3.17333E-02
 NP(BCC) =   0.5722 with U-fractions C  =  6.49332E-04
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY:
POLY:Hit RETURN to continue
POLY:
POLY:
POLY: @@ Now calculate the paraequilibrium for the steel
POLY: @@ at varying temperatures
POLY:
POLY: s-a-v 1 t 800 1200 20
   ... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex23c y
   ... the command in full is SAVE_WORKSPACES
POLY: 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/:
```

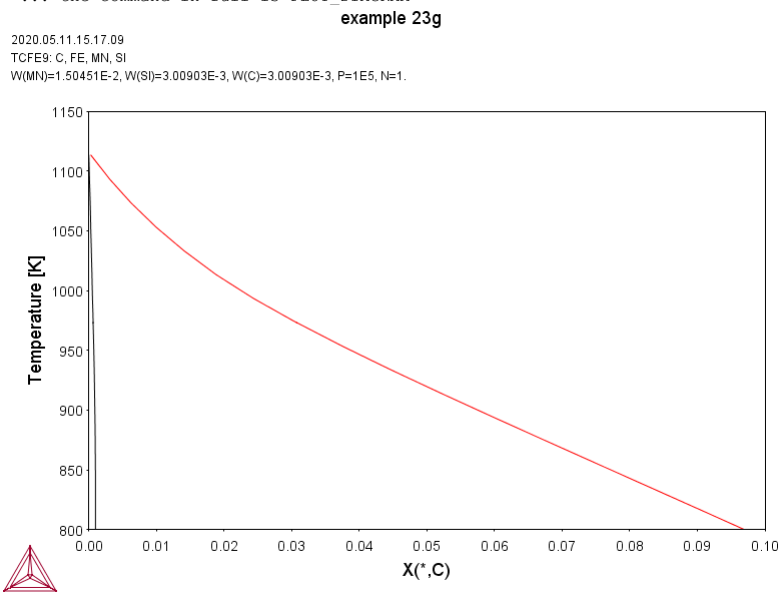
```
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    973.150     for:
     BCC_A2
     FCC_A1
   9.731500E+02    0.428    0.572   3.173334E-02   6.493319E-04  -1.294487E+00
   9.531500E+02    0.345    0.655   3.908283E-02   7.314458E-04  -8.709117E-01
   9.331500E+02    0.285    0.715   4.698896E-02   8.055430E-04  -4.580682E-01
   9.131500E+02    0.240    0.760   5.533826E-02   8.693592E-04  -5.286679E-02
   8.931500E+02    0.206    0.794   6.403695E-02   9.214025E-04   3.476768E-01
   8.731500E+02    0.180    0.820   7.300842E-02   9.607769E-04   7.462754E-01
   8.531500E+02    0.160    0.840   8.219634E-02   9.870513E-04   1.145355E+00
   8.331500E+02    0.143    0.857   9.155621E-02   1.000174E-03   1.547101E+00
   8.131500E+02    0.129    0.871   1.010626E-01   1.000393E-03   1.953500E+00
   8.000000E+02    0.122    0.878   1.073874E-01   9.937374E-04   2.224134E+00

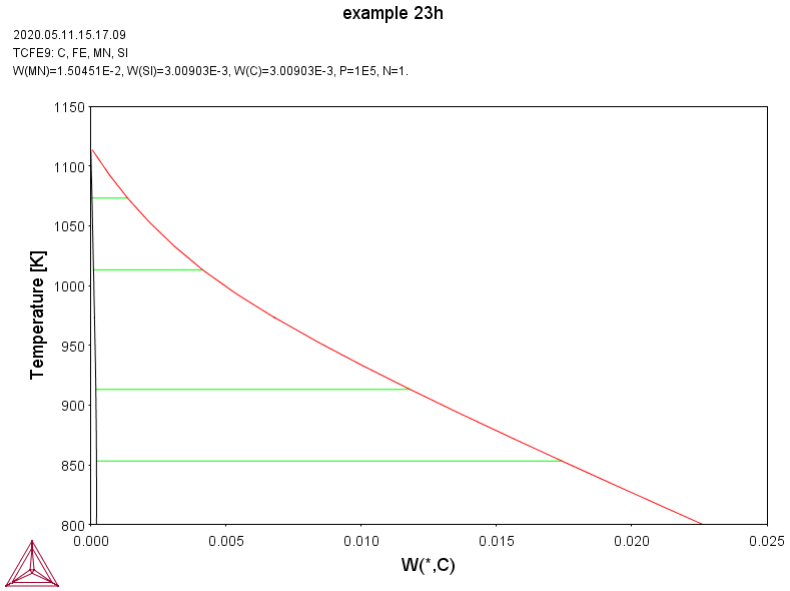
 Phase Region from    973.150     for:
     BCC_A2
     FCC_A1
   9.731500E+02    0.428    0.572   3.169255E-02   6.483345E-04  -1.296185E+00
   9.931500E+02    0.547    0.453   2.503687E-02   5.615087E-04  -1.733291E+00
   1.013150E+03    0.718    0.282   1.922949E-02   4.746917E-04  -2.184046E+00
   1.033150E+03    0.974    0.026   1.430620E-02   3.903300E-04  -2.652594E+00
   1.053150E+03    1.403   -0.403   1.003057E-02   3.030407E-04  -3.169245E+00
   1.073150E+03    2.250   -1.250   6.316751E-03   2.115347E-04  -3.783409E+00
   1.093150E+03    4.635   -3.635   3.098942E-03   1.150804E-04  -4.638490E+00
   1.113150E+03   45.149  -44.149   3.218503E-04   1.325340E-05  -7.038270E+00
 *** Buffer savend on file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex23\TCEX23~3.POL
 *** ERROR     3 IN NS01AD: Numerical error
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST:
POST: set-title example 23g
POST: s-d-a x x(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



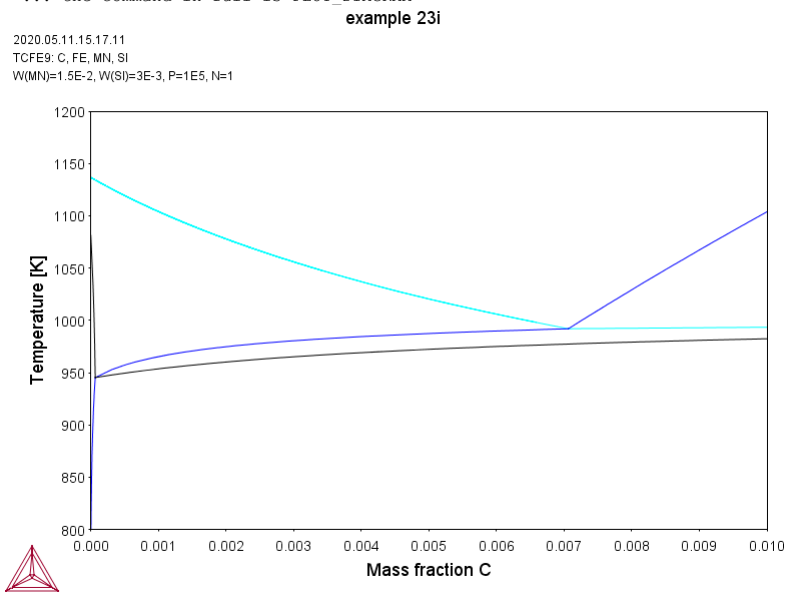

```
POST:
POST:Hit RETURN to continue
POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: s-t-s 3
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 23h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



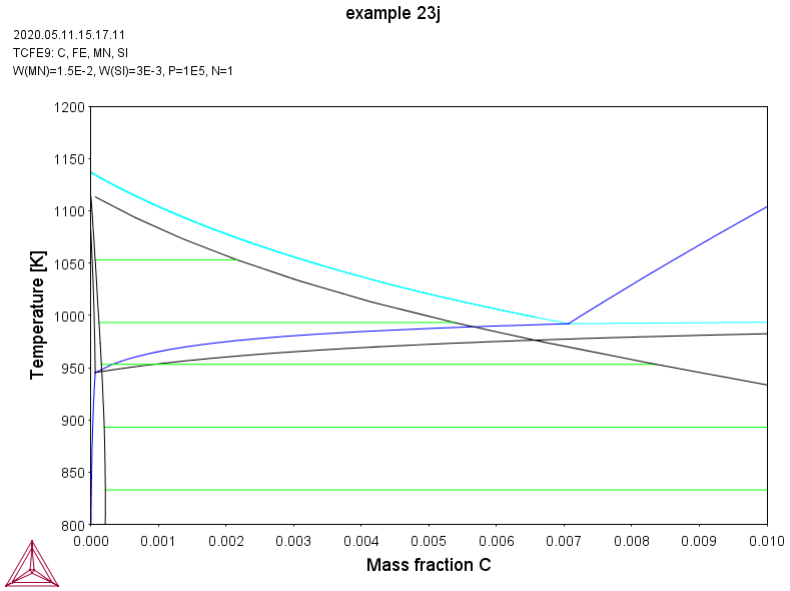

```
POST:
POST:Hit RETURN to continue
POST: make tcex23c y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: ba
   ... the command in full is BACK
POLY: read tcex23a
   ... the command in full is READ_WORKSPACES
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

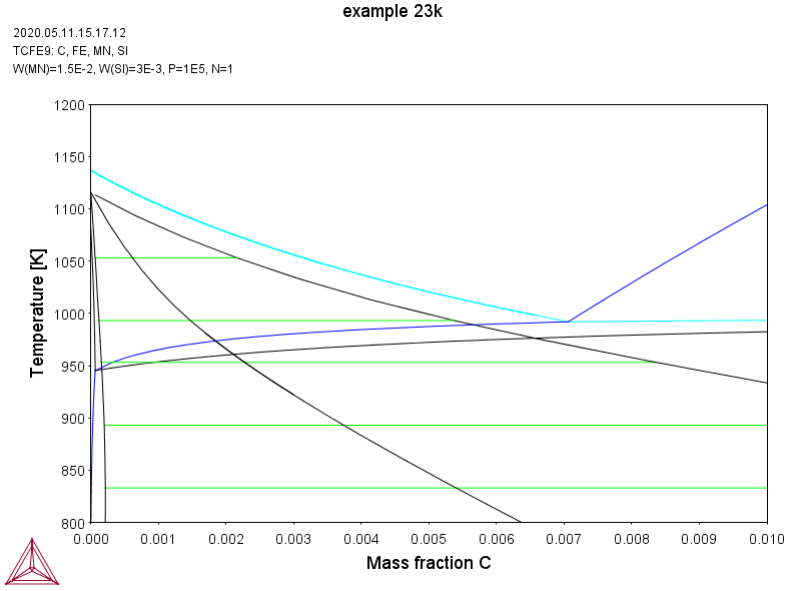
POST:
POST:
POST: set-title example 23i
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23c
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23j
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23b.exp tcex23c.exp 0; 1; 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: set-title example 23k
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY: @@ Now calculate both a normal and paraequilibrium
POLY: @@ for the steel at 1000 K.
POLY:
POLY: @@ Note that a paraequilibrium does not always exist
POLY: @@ for the given conditions. The calculated results
POLY: @@ are the amounts of the two phases. This indicates
POLY: @@ how much of the phases can be tranformed at
POLY: @@ paraequilibrium conditions. The carbon content of
POLY: @@ the phases are also listed; the other alloying
POLY: @@  elements have the same fractions in both phases
POLY:
POLY: read tcex23a.POLY3
   ... the command in full is READ_WORKSPACES
POLY: s-c T=1000
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         23291 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: l-e,,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -4.34568E+04,  Enthalpy  2.63111E+04,  Volume  7.20614E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.3754E-02  3.0000E-03 1.6697E-01 -1.4882E+04 SER
 FE                      9.6533E-01  9.7900E-01 6.1069E-03 -4.2390E+04 SER
 MN                      1.5035E-02  1.5000E-02 4.0532E-05 -8.4088E+04 SER
 SI                      5.8820E-03  3.0000E-03 3.3217E-10 -1.8147E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.3719E-01, Mass 2.9324E+01, Volume fraction 5.3039E-01  Mass fractions:
 FE  9.69680E-01  MN  2.22420E-02  C   5.52956E-03  SI  2.54842E-03

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.6281E-01, Mass 2.5743E+01, Volume fraction 4.6961E-01  Mass fractions:
 FE  9.89616E-01  MN  6.75056E-03  SI  3.51441E-03  C   1.18545E-04
POLY: 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) =   0.5975 with U-fractions C  =  2.29813E-02
 NP(BCC) =   0.4025 with U-fractions C  =  5.32466E-04
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY:
POLY:Hit RETURN to continue
POLY: @@ Now calculate an isothermal phase diagram at 1000 K
POLY: s-a-v 2 w(mn) 0 .1,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY:Hit RETURN to continue
POLY: save tcex23d y
   ... the command in full is SAVE_WORKSPACES
POLY: 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:   2.519E-03  2.500E-03
     BCC_A2
  ** CEMENTITE
     FCC_A1
 Calculated.                     11 equilibria

 Phase region boundary   2 at:   1.819E-04  1.155E-03
     BCC_A2
  ** CEMENTITE
  ** FCC_A1

 Phase region boundary   3 at:   1.819E-04  1.155E-03
     BCC_A2
  ** CEMENTITE
 Calculated                     14 equilibria

 Phase region boundary   4 at:   1.819E-04  1.155E-03
     BCC_A2
  ** FCC_A1
 Calculated                     20 equilibria
```

```
Phase region boundary   5 at:   1.819E-04  1.155E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     41 equilibria
Terminating at axis limit.

Phase region boundary   6 at:   1.819E-04  1.155E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     30 equilibria

Phase region boundary   7 at:   7.338E-03  7.005E-03
 ** BCC_A2
 ** CEMENTITE
    FCC_A1

Phase region boundary   8 at:   7.338E-03  7.005E-03
 ** CEMENTITE
    FCC_A1
Calculated..                     39 equilibria
Terminating at axis limit.

Phase region boundary   9 at:   7.338E-03  7.005E-03
 ** BCC_A2
    FCC_A1
Calculated                     40 equilibria

Phase region boundary  10 at:   7.338E-03  7.005E-03
 ** BCC_A2
    CEMENTITE
    FCC_A1
Calculated..                     13 equilibria
Terminating at axis limit.

Phase region boundary  11 at:   2.519E-03  2.500E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     21 equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   2.500E-04  5.820E-02
 ** BCC_A2
    FCC_A1
Calculated                     22 equilibria

Phase region boundary  13 at:   2.500E-04  5.820E-02
 ** BCC_A2
    FCC_A1
Calculated.                     30 equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   3.417E-03  3.132E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     14 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   3.417E-03  3.132E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     17 equilibria
Terminating at known equilibrium

Phase region boundary  16 at:   6.583E-03  6.086E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                     27 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   6.583E-03  6.086E-03
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   6.962E-03  2.500E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     29 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   6.962E-03  2.500E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     14 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   9.750E-03  3.144E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                     40 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   9.750E-03  3.144E-03
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                      3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   4.029E-03  3.417E-02
 ** BCC_A2
    FCC_A1
```

```
Calculated.                     22 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   4.029E-03  3.417E-02
 ** BCC_A2
    FCC_A1
Calculated                     34 equilibria

Phase region boundary  24 at:   7.086E-03  3.417E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     12 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   7.086E-03  3.417E-02
 ** CEMENTITE
    FCC_A1
Calculated..                     28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  26 at:   6.837E-03  6.583E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     25 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   6.837E-03  6.583E-02
 ** CEMENTITE
    FCC_A1
Calculated..                     15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:   6.837E-03  6.583E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     25 equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   6.837E-03  6.583E-02
 ** CEMENTITE
    FCC_A1
Calculated..                     15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  30 at:   6.633E-03  9.750E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     38 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   6.633E-03  9.750E-02
 ** CEMENTITE
    FCC_A1
Calculated..                      3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  32 at:   2.500E-04  5.820E-02
 ** BCC_A2
    FCC_A1
Calculated                     4 equilibria

Phase region boundary  33 at:   2.500E-04  5.820E-02
 ** BCC_A2
    FCC_A1
Calculated.                     30 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   3.417E-03  3.851E-02
 ** BCC_A2
    FCC_A1
Calculated                     26 equilibria

Phase region boundary  35 at:   3.417E-03  3.851E-02
 ** BCC_A2
    FCC_A1
Calculated.                     17 equilibria
Terminating at known equilibrium

Phase region boundary  36 at:   6.583E-03  1.379E-02
 ** BCC_A2
    FCC_A1
Calculated                     38 equilibria

Phase region boundary  37 at:   6.583E-03  1.379E-02
 ** BCC_A2
    FCC_A1
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary  38 at:   6.633E-03  9.750E-02
 ** CEMENTITE
    FCC_A1
Calculated.                     38 equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.633E-03  9.750E-02
 ** CEMENTITE
    FCC_A1
Calculated..                      3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

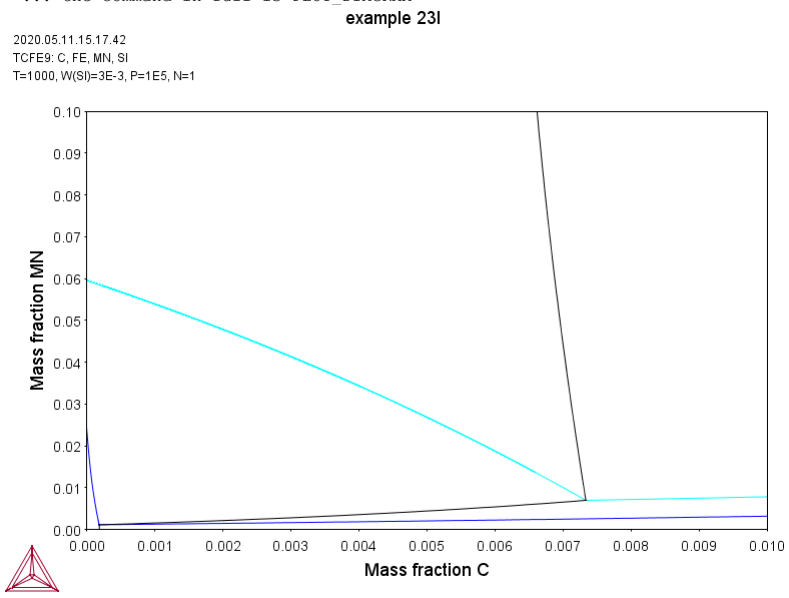
Phase region boundary  40 at:   9.750E-03  7.770E-03
 ** BCC_A2
    CEMENTITE
    FCC_A1
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   9.750E-03  7.770E-03
 ** BCC_A2
    CEMENTITE
```

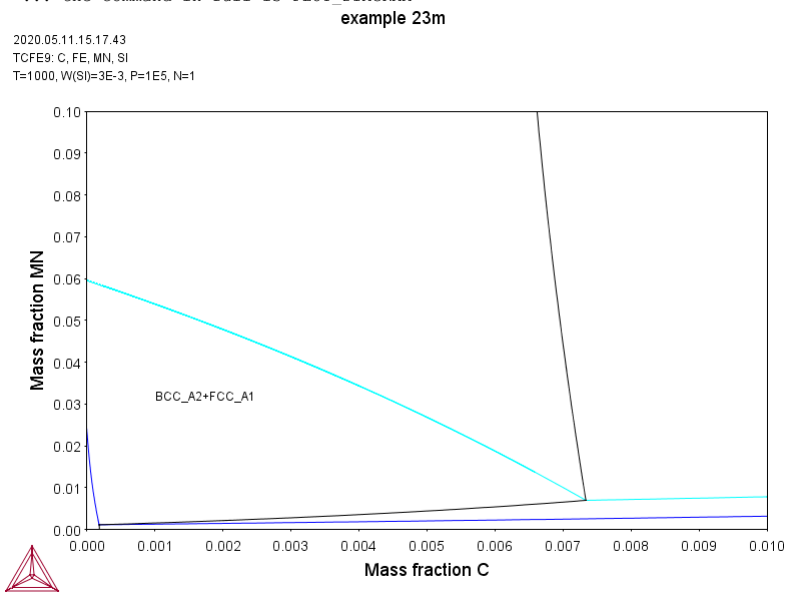
```
     FCC_A1
 Calculated..                        3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex23\tcex23d.POLY3
 CPU time for mapping                      8 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST:
POST: set-title example 23l
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: add .001 .03,,,,
   ... the command in full is ADD_LABEL_TEXT
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
 Stable phases are: BCC_A2+FCC_A1
POST: set-title example 23m
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY: @@ Calculate the corresponding paraequilibrium diagram
```

```
POLY: @@ where fcc and bcc have the same alloy composition.
POLY:
POLY: read tcex23d
   ... the command in full is READ_WORKSPACES
POLY: @@ Only one axis is set, the interstitial
POLY: @@ composition must not be an axis
POLY:
POLY: s-a-v 1 w(mn) 0 .1,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex23e y
   ... the command in full is SAVE_WORKSPACES
POLY: 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

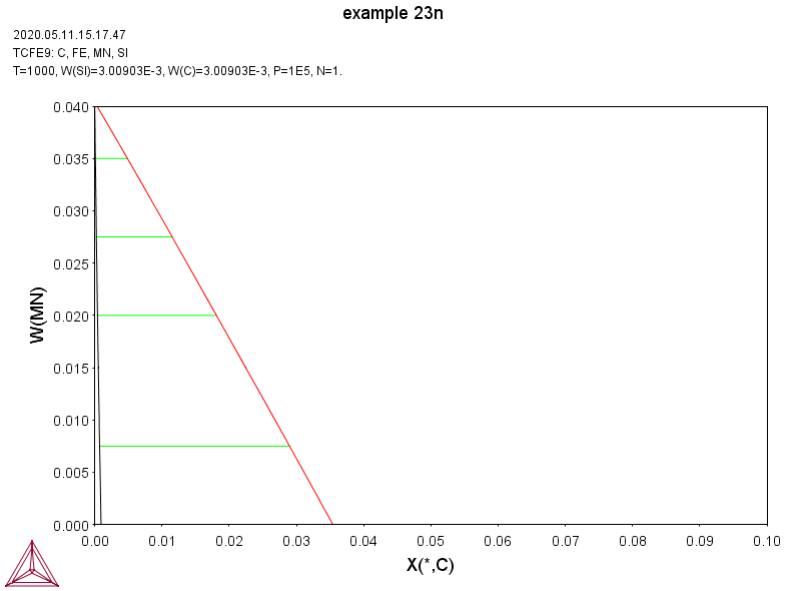
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, 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   2.298130E-02   5.324656E-04  -1.884262E+00
   1.250000E-02    0.541    0.459   2.526620E-02   5.953468E-04  -1.755801E+00
   1.000000E-02    0.494    0.506   2.755502E-02   6.602935E-04  -1.635410E+00
   7.500000E-03    0.454    0.546   2.984685E-02   7.273287E-04  -1.521849E+00
   5.000000E-03    0.420    0.580   3.214088E-02   7.964753E-04  -1.414149E+00
   2.500000E-03    0.390    0.610   3.443637E-02   8.677563E-04  -1.311537E+00
   2.500000E-09    0.363    0.637   3.673267E-02   9.411946E-04  -1.213385E+00

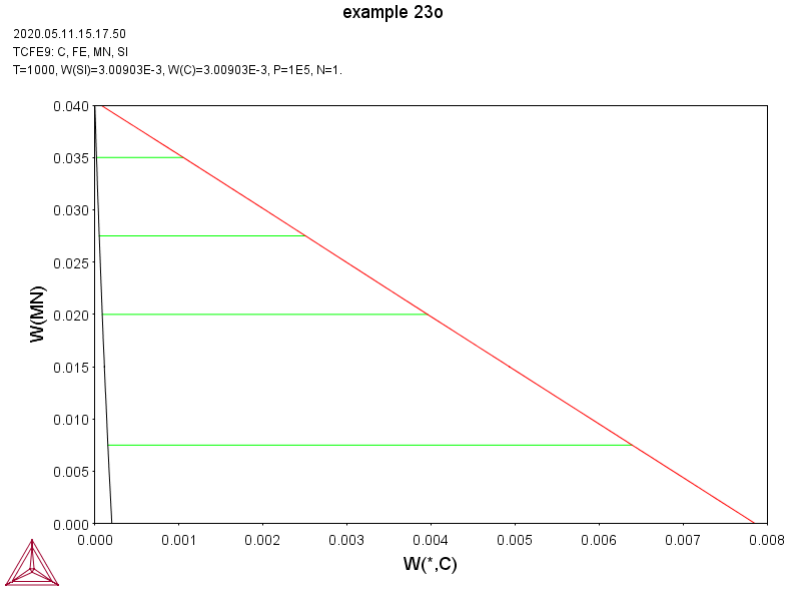
 Phase Region from   0.150000E-01 for:
     BCC_A2
     FCC_A1
   1.500000E-02    0.597    0.403   2.298507E-02   5.325999E-04  -1.883857E+00
   1.750000E-02    0.666    0.334   2.070518E-02   4.717575E-04  -2.021980E+00
   2.000000E-02    0.751    0.249   1.843132E-02   4.129355E-04  -2.171954E+00
   2.250000E-02    0.860    0.140   1.616471E-02   3.561118E-04  -2.336785E+00
   2.500000E-02    1.003   -0.003   1.390672E-02   3.012642E-04  -2.520810E+00
   2.750000E-02    1.201   -0.201   1.165633E-02   2.483135E-04  -2.730865E+00
   3.000000E-02    1.493   -0.493   9.403448E-03   1.969802E-04  -2.979205E+00
   3.250000E-02    1.971   -0.971   7.146659E-03   1.471949E-04  -3.287293E+00
   3.500000E-02    2.894   -1.894   4.884299E-03   9.890192E-05  -3.701654E+00
   3.750000E-02    5.421   -4.421   2.615000E-03   5.205229E-05  -4.360257E+00
   4.000000E-02   42.148  -41.148   3.373209E-04   6.599705E-06  -6.442195E+00
 *** Buffer savend on file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex23\TC9F56~1.POL
 *** ERROR     7 IN NS01AD: Numerical error
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST:
POST: s-t-s 3
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 23n
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



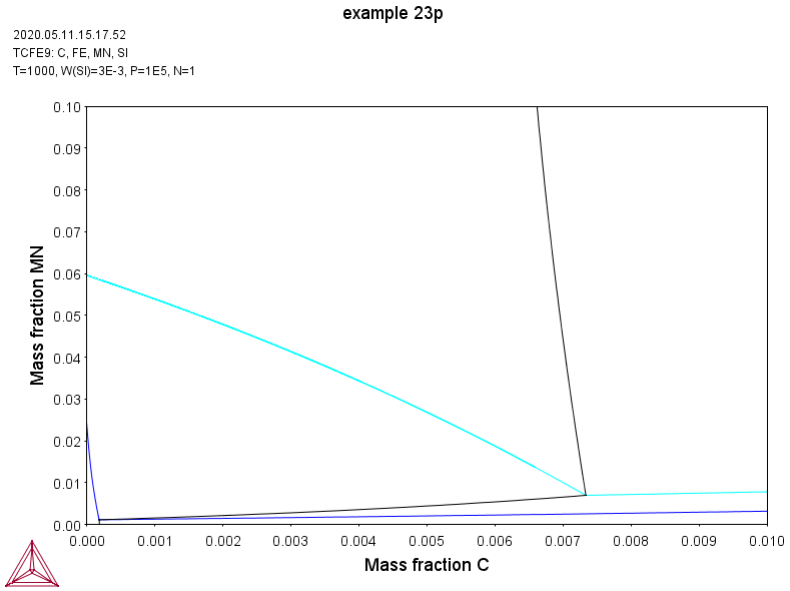

```
POST:
POST:Hit RETURN to continue
POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: set-title example 23o
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



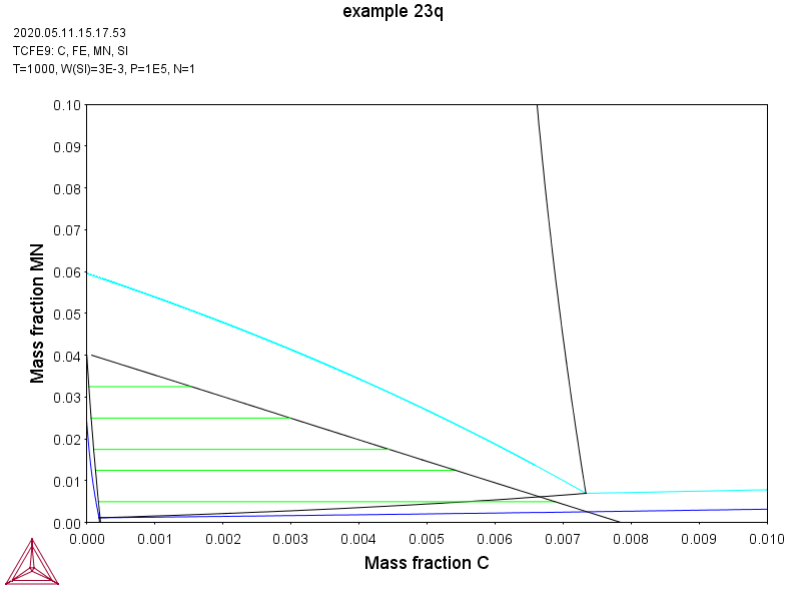

```
POST:
POST: make tcex23e y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY: @@ Now overlay the two diagrams
POLY: read tcex23d
   ... the command in full is READ_WORKSPACES
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST:
POST: set-title example 23p
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex23e
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 23q
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex24

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex24\tcex24.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Simulation of the silicon arc furnace using the REACTOR module
SYS:
SYS: @@ This is a simple reactor model with output of gases at the top
SYS: @@ and output of condensed phases at the bottom. The gas phase
SYS: @@ from one segment flows to higher segments, 80% reacts in the
SYS: @@ first above, 15% in the second above and 5 % in the third
SYS: @@ above. The condensed phases flow downwards and all of it goes
SYS: @@ to the next lowest segment.
SYS:
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
SYS: @@ specify the heat content.
SYS:
SYS: @@ Note that a SSUB database license is required to run
SYS: @@ the example.
SYS:
SYS: @@ First fetch data
SYS: GO DAT
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: SW SSUB6
 Current database: SGTE Substances Database v6.0

 VA  DEFINED
TDB_SSUB6:
TDB_SSUB6: @@ Define-species means that data for just these species is
TDB_SSUB6: @@ retrieved. Define-system means that data for all
TDB_SSUB6: @@ combinations of the elements would be retrieved and this
TDB_SSUB6: @@ is not necessary.
TDB_SSUB6:
TDB_SSUB6: DEF-SPECIES C C1O1 C1O2 C1SI1 C2 C3 N1O1 N2 N4SI3
 C                       C1O1                    C1O2
 C1SI1                   C2                      C3
 N1O1                    N2                      N4SI3
   DEFINED
TDB_SSUB6: DEF-SP O O2 SI O1SI1 O2SI1
 O                       O2                      SI
 O1SI1                   O2SI1  DEFINED
TDB_SSUB6: GET
15:19:15,791 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
      C1<G> C<G>
   C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      C1O1<G> CO<G>
      CARBON MONOXIDE <GAS>
      STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
   C1O2<G> T.C.R.A.S. Class: 2
      C1O2<G> CO2<G>
      CARBON DIOXIDE <GAS>
   C1SI1<G> T.C.R.A.S. Class: 5
      C1SI1<G> SiC<G>
      SILICON CARBIDE <GAS>
   C2<G> T.C.R.A.S. Class: 2
      CARBON Diatomic Gas.
      CARBON <DIATOMIC GAS>
   C3<G> T.C.R.A.S. Class: 6
      CARBON triatomic gas.
      CARBON <TRIATOMIC GAS>
   N1O1<G> T.C.R.A.S. Class: 1
      N1O1<G> NO<G>
      NITRIC OXIDE <GAS>
   N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      N2<G> N2<G>
      NITROGEN <DIATOMIC GAS>
      PUBLISHED BY JANAF AT 09/65
   O1<G> TCRAS 02/06/80
      O1 Gaseous Standard State.
   O1SI1<G> T.C.R.A.S. Class: 1
      O1SI1<G> SiO<G>
      SILICON <MONOXIDE GAS>
   O2<G> TCRAS 21/06/90
      OXYGEN Gaseous Standard State.
   O2SI1<G> T.C.R.A.S. Class: 5
      O2SI1<G> SiO2<G>
      SILICON DIOXIDE <GAS>
   SI1<G> T.C.R.A.S. Class: 1
      SI1<G> Si<G>
      SILICON <GAS>
   O2SI1<BETA-QUARTZ> N.P.L.
      O2SI1<BETA_QUARTZ> SiO2<BETA_QUARTZ>
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
```

```
      system by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   C1SI1<ALPHA> JANAF THERMOCHEMICAL TABLES SGTE **
      C1SI1<C1SI1_ALPHA> SiC<ALPHA>
      N CARBIDE <ALPHA>
      ALPHA-SIC . HEX.FORM . PUBL. BY JANAF AT 3/67 .LESS STABLE THAN
      SIC_BETA UP TO 2200K. Decomposes to complex vapour at about 3259K.
   C1SI1<BETA> JANAF THERMOCHEMICAL TABLES SGTE
      C1SI1<C1SI1_BETA> SiC<BETA>
      N CARBIDE <BETA>
      CUBIC FORM OF TYPE ZNS. STABLE WITH RESPECT TO SIC-ALPHA UP TO 2200K.
      PUBL. BY JANAF 03/67
   O2SI1<CRISTOBALITE> N.P.L.
      O2SI1<CRISTOBALITE> SiO2<CRISTOBALITE>
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   C1 S.G.T.E. **
      GRAPHITE
      Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
   C1<DIAMOND> S.G.T.E. **
      C1<DIAMOND> <DIAMOND>
      DIAMOND
      Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
      from 1994 database (ex THERMODATA 01/93)
   N4SI3 CHATILLON(1997)
      N4SI3 Si3N4 N4SI3
      Gurvich V.V., Veyts I.V., Alcock C.B., Thermodynamical Properties of
      Individual Substances,4th ed. Vol 1 and 2 English Ed (1990). S(298)
      corrected according to Koshchenko V.I., Grindberg Ya. Zh. Inorg.
      Mater.
      18(6) 903-5 (1982). Recent calorimetric determination par O'Hare et
      al., J. Mater. Res., 12 (1997) 3203-3205. Enthalpy of transformation
      alpha to beta very small(1 +- 4 kJ/ mol ) but no knowledge of T trans.
      according to them.
   O2SI1<L> N.P.L.
      O2SI1<LIQUID_O2SI> SiO2<LIQUID>
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   O2SI1<QUARTZ> N.P.L.
      O2SI1<QUARTZ> SIO2<QUARTZ> SiO2<quartz>
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   SI1 JANAF THERMOCHEMICAL TABLES SGTE **
      SI1 Si
      SILICON
      PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
      --U.D. 31/10/85
   O2SI1<TRIDYMITE> N.P.L.
      O2SI1<TRIDYMITE> SIO2<TRIDYMITE> SiO2<TRIDYMITE>
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
 -OK-
TDB_SSUB6: GO G
 GIBBS ENERGY SYSTEM
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 N4SI3_S                    82200000     1
  10 O2SI1_L                    82200000     1
  11 O2SI1_QUARTZ               82200000     1
  12 O2SI1_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
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
REACTOR: @@ graphite (C) is added. A small amount of N is also added to
REACTOR: @@ simplify calculations. 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
REACTOR: @@ provided.
REACTOR:
REACTOR: CREATE_STAGE
NUMBER OF STAGE BOXES /4/: 4
 YOU MUST FIRST DEFINE FEED FROM SURROUNDINGS!
GIVE FEED TO SYSTEM: N(C)=1.8
Input temperature /298.15/:
GIVE FEED TO SYSTEM: N(O2SI1)=1
Input temperature /298.15/:
GIVE FEED TO SYSTEM: H=876000
GIVE FEED TO SYSTEM: N(N2)=4e-4
Input temperature /298.15/:
GIVE FEED TO SYSTEM:

 GIVE FOR STAGE BOX     1
NAME: /SEGMENT_1/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 1750
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

 GIVE FOR STAGE BOX     2
NAME: /SEGMENT_2/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 1900
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

 GIVE FOR STAGE BOX     3
NAME: /SEGMENT_3/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 2050
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

 GIVE FOR STAGE BOX     4
NAME: /SEGMENT_4/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 2200
Give initial amount:
 Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST
REACTOR: l-r

 Number:  0 name: SURROUNDINGS            stage box at:    23,
 Feed of C                       with  1.8000E+00 mol to record:    -1
 Feed of O2SI1                   with  1.0000E+00 mol to record:    -1
 Feed of heat  8.7600E+05 J to record:    -1
 Feed of N2                      with  4.0000E-04 mol to record:    -1

 Number:  1 name: SEGMENT_1               stage box at:    72, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:  2 name: SEGMENT_2               stage box at:   114, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:  3 name: SEGMENT_3               stage box at:   156, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1

 Number:  4 name: SEGMENT_4               stage box at:   198, H controlled
 Output for phase GAS                     to record:   -1
 Output for phase REST                    to record:   -1
REACTOR: @@ Create dividers, one for distributing the gas from segment
REACTOR: @@ 2 to 4, one for splitting the heat feed, and one for splitting
REACTOR: @@ the feed on N2
REACTOR:
REACTOR: create-div
Number of dividers /4/: 5
Number of outputs for divider 1: /3/: 2
Percent of input to output 1: /100/: 80
Number of outputs for divider 2: /3/: 3
Percent of input to output 1: /100/: 80 15
Number of outputs for divider 3: /3/: 3
Percent of input to output 1: /100/: 80 15
Number of outputs for divider 4: /3/: 3
Percent of input to output 1: /100/: 85 10
Number of outputs for divider 5: /3/: 4
Percent of input to output 1: /100/: 25 25 25
```

```
REACTOR: l-r

 Number:  0 name: SURROUNDINGS             stage box at:    23,
 Feed of C                        with  1.8000E+00 mol to record:    -1
 Feed of O2SI1                    with  1.0000E+00 mol to record:    -1
 Feed of heat  8.7600E+05 J to record:    -1
 Feed of N2                       with  4.0000E-04 mol to record:    -1

 Number:  1 name: SEGMENT_1                stage box at:    72, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:  2 name: SEGMENT_2                stage box at:   114, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:  3 name: SEGMENT_3                stage box at:   156, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:  4 name: SEGMENT_4                stage box at:   198, H controlled
 Output for phase GAS                      to record:   -1
 Output for phase REST                     to record:   -1

 Number:   5 name: DIVIDER_5                divider at:   240
   80 % of input to record:   -1
   20 % of input to record:   -1

 Number:   6 name: DIVIDER_6                divider at:   268
   80 % of input to record:   -1
   15 % of input to record:   -1
    5 % of input to record:   -1

 Number:   7 name: DIVIDER_7                divider at:   301
   80 % of input to record:   -1
   15 % of input to record:   -1
    5 % of input to record:   -1

 Number:   8 name: DIVIDER_8                divider at:   334
   85 % of input to record:   -1
   10 % of input to record:   -1
    5 % of input to record:   -1

 Number:   9 name: DIVIDER_9                divider at:   367
   25 % of input to record:   -1
   25 % of input to record:   -1
   25 % of input to record:   -1
   25 % of input to record:   -1
REACTOR: @@ Finally create the pipes between the segments first for the feed
REACTOR: c-pipe 0 1 1 8 9
 Feed of C
 Feed of O2SI1
 Feed of heat
 Input set to this divider
 Feed of N2
 Input set to this divider
 NO MORE OUTPUT RECORDS
REACTOR: @@ All solid phases are assumed to go down one segment
REACTOR: @@ The gas phase is assumed to go up, 80% to the next segment,
REACTOR: @@ 15% to the second next and 5% to the third segment above.
REACTOR: @@ Output from stage boxes
REACTOR:
REACTOR: c-pipe 1 0 2
 Output record for phase GAS
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 2 5 3
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 3 6 4
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 4 7 0
 Output record for phase GAS
 Input set to this divider
 Output record for phase REST
 NO MORE OUTPUT RECORDS
REACTOR: @@ Output from dividers
REACTOR: c-pipe 5 1 0
 Output record for   80 % of input
 Output record for   20 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 6 2 1 0
 Output record for   80 % of input
 Output record for   15 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 7 3 2 1
 Output record for   80 % of input
 Output record for   15 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 8 4 3 2
 Output record for   85 % of input
 Output record for   10 % of input
 Output record for    5 % of input
 NO MORE OUTPUT RECORDS
REACTOR: c-pipe 9 1 2 3 4
 Output record for   25 % of input
 Output record for   25 % of input
 Output record for   25 % of input
 Output record for   25 % of input
 NO MORE OUTPUT RECORDS
REACTOR: l-r

 Number:  0 name: SURROUNDINGS             stage box at:    23,
 Feed of C                        with  1.8000E+00 mol to record:     1
 Feed of O2SI1                    with  1.0000E+00 mol to record:     1
 Feed of heat  8.7600E+05 J to record:     8
 Feed of N2                       with  4.0000E-04 mol to record:     9
```

```
 Number:  1 name: SEGMENT_1                stage box at:    72, H controlled
 Output for phase GAS                      to record:    0
 Output for phase REST                     to record:    2

 Number:  2 name: SEGMENT_2                stage box at:   114, H controlled
 Output for phase GAS                      to record:    5
 Output for phase REST                     to record:    3

 Number:  3 name: SEGMENT_3                stage box at:   156, H controlled
 Output for phase GAS                      to record:    6
 Output for phase REST                     to record:    4

 Number:  4 name: SEGMENT_4                stage box at:   198, H controlled
 Output for phase GAS                      to record:    7
 Output for phase REST                     to record:    0

 Number:   5 name: DIVIDER_5                divider at:   240
   80 % of input to record:    1
   20 % of input to record:    0

 Number:   6 name: DIVIDER_6                divider at:   268
   80 % of input to record:    2
   15 % of input to record:    1
    5 % of input to record:    0

 Number:   7 name: DIVIDER_7                divider at:   301
   80 % of input to record:    3
   15 % of input to record:    2
    5 % of input to record:    1

 Number:   8 name: DIVIDER_8                divider at:   334
   85 % of input to record:    4
   10 % of input to record:    3
    5 % of input to record:    2

 Number:   9 name: DIVIDER_9                divider at:   367
   25 % of input to record:    1
   25 % of input to record:    2
   25 % of input to record:    3
   25 % of input to record:    4
REACTOR: save tcex24 y
REACTOR: @@ Now start the process
REACTOR: read tcex24
REACTOR:
REACTOR: @@ The output for each iteration consists of the conditions set in
REACTOR: @@ each segment, and you can also select some state variables,
REACTOR: @@ in this case NP($) meaning moles of stable phases.
REACTOR: @@ After each loop the temperatures in all segments are listed
REACTOR:
REACTOR: @@ We want to achive a reactor where only Si<L> leaves at the bottom.
REACTOR: START
Max number of loops: /10/: 50
OUTPUT TO SCREEN OR FILE /SCREEN/:
Output conditions? /Y/:
Output variables: /T BP($)/: T BP($)
 >>> DATA AT ITERATION     1 FROM STAGE    1
 T=1750, P=1E5, N(C)=1.8, N(N)=2E-4, N(O)=2, N(SI)=1
 DEGREES OF FREEDOM 0
T= 1.750000E+03
 BP(GAS)=8.3899239E-3, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=3.9560636E-3, BP(CRISTOBALITE)=60.077021, BP(C_L)=0,
    BP(C_S)=21.616235, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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(N4SI3_S)=0, BP(O2SI1_L)=22.396537, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_QUARTZ_S2)=0, BP(SI_L)=6.3106228E-4, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION    1 FROM STAGE    4
 T=2200, P=1E5, N(C)=0.586424, N(N)=2E-4, N(O)=0.74552, N(SI)=0.959207
 DEGREES OF FREEDOM 0
T= 2.200000E+03
 BP(GAS)=27.369406, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=9.7781171, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_QUARTZ_S2)=0, BP(SI_L)=8.7657159, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    2 FROM STAGE    1
 H=-9.69232E5, P=1E5, N(C)=2.78779, N(N)=4E-4, N(O)=3.04056, N(SI)=1.0527
 DEGREES OF FREEDOM 0
T= 1.098651E+03
 BP(GAS)=25.395955, BP(BETA_QUARTZ)=63.249404, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=0, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=23.055463,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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)=2.5771879E-2, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=0.19891753, BP(CRISTOBALITE)=66.592185, BP(C_L)=0,
    BP(C_S)=23.605007, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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)=28.121362, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
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    BP(C1SI1_BETA)=21.054185, BP(CRISTOBALITE)=54.435284, BP(C_L)=0,
    BP(C_S)=8.6836041, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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)=60.210326, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=0.55847707, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_QUARTZ_S2)=0, BP(SI_L)=23.407071, BP(SI_S)=0, BP(TRIDYMITE)=0,
    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    3 FROM STAGE    1
 H=-9.22751E5, P=1E5, N(C)=2.01172, N(N)=5.76E-4, N(O)=2.24134, N(SI)=1.02991
 DEGREES OF FREEDOM 0
T= 8.124883E+02
 BP(GAS)=4.0693569, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=23.005715, BP(DIAMOND)=0,
    BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=61.879868,
    BP(O2SI1_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    3 FROM STAGE    2
 H=-9.0397E5, P=1E5, N(C)=2.89749, N(N)=5.18E-4, N(O)=3.13248, N(SI)=1.12129
 DEGREES OF FREEDOM 0
T= 1.746338E+03
 BP(GAS)=25.042951, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=67.278274, BP(C_L)=0, BP(C_S)=24.095798, BP(DIAMOND)=0,
    BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    3 FROM STAGE    3
 H=-8.04917E5, P=1E5, N(C)=2.99345, N(N)=3.6E-4, N(O)=3.68911, N(SI)=1.58674
 DEGREES OF FREEDOM 0
T= 1.785838E+03
 BP(GAS)=55.589668, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=28.960504, BP(CRISTOBALITE)=51.37138, BP(C_L)=0,
    BP(C_S)=3.6235824, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    3 FROM STAGE    4
 H=61307.1, P=1E5, N(C)=1.02397, N(N)=2E-4, N(O)=1.71001, N(SI)=1.57729
 DEGREES OF FREEDOM 0
T= 2.594647E+03
 BP(GAS)=59.391022, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=24.567245, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    4 FROM STAGE    1
 H=-9.75673E5, P=1E5, N(C)=2.8597, N(N)=6.784E-4, N(O)=3.09674, N(SI)=1.03777
 DEGREES OF FREEDOM 0
T= 1.067994E+03
 BP(GAS)=27.303365, BP(BETA_QUARTZ)=62.352571, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=0, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=23.392027,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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    4 FROM STAGE    2
 H=-9.26156E5, P=1E5, N(C)=3.67673, N(N)=5.18E-4, N(O)=3.91533, N(SI)=1.15072
 DEGREES OF FREEDOM 0
T= 1.785833E+03
 BP(GAS)=48.987037, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=2.2730167, BP(CRISTOBALITE)=65.232008, BP(C_L)=0,
    BP(C_S)=22.635726, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    4 FROM STAGE    3
 H=-7.59974E5, P=1E5, N(C)=2.76045, N(N)=3.6E-4, N(O)=3.53941, N(SI)=1.70442
 DEGREES OF FREEDOM 0
T= 1.856422E+03
 BP(GAS)=54.420155, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.739066, BP(CRISTOBALITE)=48.497149, BP(C_L)=0,
    BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    4 FROM STAGE    4
 H=97718.1, P=1E5, N(C)=0.866397, N(N)=2E-4, N(O)=1.61434, N(SI)=1.67357
 DEGREES OF FREEDOM 0
T= 2.773504E+03
 BP(GAS)=58.669424, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=24.569593, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    5 FROM STAGE    1
 H=-1.01358E6, P=1E5, N(C)=3.5158, N(N)=6.784E-4, N(O)=3.76462, N(SI)=1.05123
 DEGREES OF FREEDOM 0
T= 1.163508E+03
 BP(GAS)=45.980219, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=22.850503, BP(DIAMOND)=0,
    BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=63.161004
 >>> DATA AT ITERATION    5 FROM STAGE    2
 H=-9.1327E5, P=1E5, N(C)=3.54766, N(N)=5.18E-4, N(O)=3.88466, N(SI)=1.19572
 DEGREES OF FREEDOM 0
T= 1.785833E+03
 BP(GAS)=49.603255, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=5.1279345, BP(CRISTOBALITE)=63.651652, BP(C_L)=0,
    BP(C_S)=19.968004, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    5 FROM STAGE    3
 H=-7.20023E5, P=1E5, N(C)=2.48349, N(N)=3.6E-4, N(O)=3.41026, N(SI)=1.82628
 DEGREES OF FREEDOM 0
T= 1.974923E+03
 BP(GAS)=54.11176, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=33.932787, BP(CRISTOBALITE)=47.641383, BP(C_L)=0,
    BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    5 FROM STAGE    4
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 H=1.21546E5, P=1E5, N(C)=0.846289, N(N)=2E-4, N(O)=1.58585, N(SI)=1.63921
 DEGREES OF FREEDOM 0
T= 2.880121E+03
 BP(GAS)=58.994116, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.582856, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    6 FROM STAGE    1
 H=-1.01075E6, P=1E5, N(C)=3.49373, N(N)=6.784E-4, N(O)=3.76565,
    N(SI)=1.07656
 DEGREES OF FREEDOM 0
T= 1.245814E+03
 BP(GAS)=44.984991, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=22.786504, BP(DIAMOND)=0,
    BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=64.683179
 >>> DATA AT ITERATION    6 FROM STAGE    2
 H=-9.07819E5, P=1E5, N(C)=3.33384, N(N)=5.18E-4, N(O)=3.85053, N(SI)=1.35148
 DEGREES OF FREEDOM 0
T= 1.785834E+03
 BP(GAS)=49.986925, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=12.328795, BP(CRISTOBALITE)=62.215898, BP(C_L)=0,
    BP(C_S)=15.079393, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    6 FROM STAGE    3
 H=-6.89982E5, P=1E5, N(C)=2.23998, N(N)=3.6E-4, N(O)=3.33968, N(SI)=2.01108
 DEGREES OF FREEDOM 0
T= 2.024859E+03
 BP(GAS)=55.901308, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=33.947222, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=46.973649, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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    6 FROM STAGE    4
 H=1.42732E5, P=1E5, N(C)=0.846649, N(N)=2E-4, N(O)=1.56363, N(SI)=1.62846
 DEGREES OF FREEDOM 0
T= 2.939413E+03
 BP(GAS)=59.078725, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=21.844948, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    7 FROM STAGE    1
 H=-1.00894E6, P=1E5, N(C)=3.46804, N(N)=6.784E-4, N(O)=3.76822,
    N(SI)=1.10673
 DEGREES OF FREEDOM 0
T= 1.360090E+03
 BP(GAS)=43.509997, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=23.028873, BP(DIAMOND)=0,
    BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=66.495403
 >>> DATA AT ITERATION    7 FROM STAGE    2
 H=-9.0846E5, P=1E5, N(C)=3.15898, N(N)=5.18E-4, N(O)=3.86884, N(SI)=1.54042
 DEGREES OF FREEDOM 0
T= 1.785834E+03
 BP(GAS)=51.714963, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=20.759109, BP(CRISTOBALITE)=60.91749, BP(C_L)=0,
    BP(C_S)=9.7183714, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    7 FROM STAGE    3
 H=-6.68401E5, P=1E5, N(C)=2.00418, N(N)=3.6E-4, N(O)=3.27868, N(SI)=2.21214
 DEGREES OF FREEDOM 0
T= 2.054719E+03
 BP(GAS)=58.391064, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.178134, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=46.091554, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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    7 FROM STAGE    4
 H=1.5752E5, P=1E5, N(C)=0.852408, N(N)=2E-4, N(O)=1.53426, N(SI)=1.61954
 DEGREES OF FREEDOM 0
T= 2.970399E+03
 BP(GAS)=58.350805, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=21.921685, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    8 FROM STAGE    1
 H=-1.01026E6, P=1E5, N(C)=3.48108, N(N)=6.784E-4, N(O)=3.81122,
    N(SI)=1.13788
 DEGREES OF FREEDOM 0
T= 1.482989E+03
 BP(GAS)=43.00392, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=23.382924, BP(DIAMOND)=0,
    BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=68.366927
 >>> DATA AT ITERATION    8 FROM STAGE    2
 H=-9.10878E5, P=1E5, N(C)=2.99607, N(N)=5.18E-4, N(O)=3.90142, N(SI)=1.7378
 DEGREES OF FREEDOM 0
T= 1.785834E+03
 BP(GAS)=53.791867, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=29.488661, BP(CRISTOBALITE)=59.674774, BP(C_L)=0,
    BP(C_S)=4.2628222, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    8 FROM STAGE    3
 H=-6.55233E5, P=1E5, N(C)=1.77229, N(N)=3.6E-4, N(O)=3.21382, N(SI)=2.39985
 DEGREES OF FREEDOM 0
T= 2.072919E+03
 BP(GAS)=59.871551, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.480045, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=45.758107, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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    8 FROM STAGE    4
 H=1.63921E5, P=1E5, N(C)=0.859937, N(N)=2E-4, N(O)=1.52316, N(SI)=1.62152
 DEGREES OF FREEDOM 0
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T= 2.980408E+03
 BP(GAS)=57.971021, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.269932, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION    9 FROM STAGE    1
 H=-1.01265E6, P=1E5, N(C)=3.50442, N(N)=6.784E-4, N(O)=3.86176, N(SI)=1.1655
 DEGREES OF FREEDOM 0
T= 1.587698E+03
 BP(GAS)=42.882392, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=23.711015, BP(DIAMOND)=0,
    BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=70.024972
 >>> DATA AT ITERATION    9 FROM STAGE    2
 H=-9.13276E5, P=1E5, N(C)=2.83298, N(N)=5.18E-4, N(O)=3.91194, N(SI)=1.91242
 DEGREES OF FREEDOM 0
T= 1.813659E+03
 BP(GAS)=54.528551, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=36.500133, BP(CRISTOBALITE)=59.302998, BP(C_L)=0,
    BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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    9 FROM STAGE    3
 H=-6.54501E5, P=1E5, N(C)=1.59827, N(N)=3.6E-4, N(O)=3.19257, N(SI)=2.56019
 DEGREES OF FREEDOM 0
T= 2.082775E+03
 BP(GAS)=61.270688, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.761698, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=46.150363, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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    9 FROM STAGE    4
 H=1.60038E5, P=1E5, N(C)=0.866962, N(N)=2E-4, N(O)=1.53622, N(SI)=1.63507
 DEGREES OF FREEDOM 0
T= 2.968716E+03
 BP(GAS)=58.16585, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.749012, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   10 FROM STAGE    1
 H=-1.01175E6, P=1E5, N(C)=3.49117, N(N)=6.784E-4, N(O)=3.87559,
    N(SI)=1.19209
 DEGREES OF FREEDOM 0
T= 1.688378E+03
 BP(GAS)=41.819001, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=24.015589, BP(DIAMOND)=0,
    BP(N4SI3_S)=0, BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=71.592748
 >>> DATA AT ITERATION   10 FROM STAGE    2
 H=-9.17571E5, P=1E5, N(C)=2.71456, N(N)=5.18E-4, N(O)=3.93864, N(SI)=2.05542
 DEGREES OF FREEDOM 0
T= 1.931654E+03
 BP(GAS)=54.443862, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.245342, BP(CRISTOBALITE)=61.663362, BP(C_L)=0,
    BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   10 FROM STAGE    3
 H=-6.75806E5, P=1E5, N(C)=1.62247, N(N)=3.6E-4, N(O)=3.28158, N(SI)=2.61526
 DEGREES OF FREEDOM 0
T= 2.082796E+03
 BP(GAS)=62.678066, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.07906, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=47.687059, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   10 FROM STAGE    4
 H=1.40325E5, P=1E5, N(C)=0.874877, N(N)=2E-4, N(O)=1.58737, N(SI)=1.66856
 DEGREES OF FREEDOM 0
T= 2.917962E+03
 BP(GAS)=59.278419, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=23.490502, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   11 FROM STAGE    1
 H=-1.00311E6, P=1E5, N(C)=3.3844, N(N)=6.784E-4, N(O)=3.84233, N(SI)=1.26378
 DEGREES OF FREEDOM 0
T= 1.785825E+03
 BP(GAS)=40.181408, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=2.0429771, BP(CRISTOBALITE)=72.460052, BP(C_L)=0,
    BP(C_S)=22.941885, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   11 FROM STAGE    2
 H=-9.22617E5, P=1E5, N(C)=2.69033, N(N)=5.18E-4, N(O)=4.00547, N(SI)=2.13913
 DEGREES OF FREEDOM 0
T= 1.964263E+03
 BP(GAS)=56.690326, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.355783, BP(CRISTOBALITE)=62.435823, BP(C_L)=0,
    BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   11 FROM STAGE    3
 H=-6.99253E5, P=1E5, N(C)=1.63156, N(N)=3.6E-4, N(O)=3.34822, N(SI)=2.63654
 DEGREES OF FREEDOM 0
T= 2.082357E+03
 BP(GAS)=62.812323, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.943937, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=49.460881, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   11 FROM STAGE    4
 H=1.17365E5, P=1E5, N(C)=0.871507, N(N)=2E-4, N(O)=1.64642, N(SI)=1.69472
 DEGREES OF FREEDOM 0
T= 2.855981E+03
 BP(GAS)=60.986548, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
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    BP(SI_L)=23.421073, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   12 FROM STAGE    1
 H=-1.00345E6, P=1E5, N(C)=3.36452, N(N)=6.784E-4, N(O)=3.87931,
    N(SI)=1.31896
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=41.745844, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=4.6200258, BP(CRISTOBALITE)=71.897831, BP(C_L)=0,
    BP(C_S)=21.265337, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   12 FROM STAGE    2
 H=-9.23112E5, P=1E5, N(C)=2.62448, N(N)=5.18E-4, N(O)=4.00169, N(SI)=2.19444
 DEGREES OF FREEDOM 0
T= 1.981583E+03
 BP(GAS)=56.956866, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.363041, BP(CRISTOBALITE)=62.863929, BP(C_L)=0,
    BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   12 FROM STAGE    3
 H=-7.19679E5, P=1E5, N(C)=1.62905, N(N)=3.6E-4, N(O)=3.4097, N(SI)=2.66675
 DEGREES OF FREEDOM 0
T= 2.082497E+03
 BP(GAS)=63.219191, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.784905, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=51.014914, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   12 FROM STAGE    4
 H=97299.2, P=1E5, N(C)=0.867541, N(N)=2E-4, N(O)=1.69815, N(SI)=1.71661
 DEGREES OF FREEDOM 0
T= 2.791245E+03
 BP(GAS)=62.594967, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=23.207654, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   13 FROM STAGE    1
 H=-1.00205E6, P=1E5, N(C)=3.31172, N(N)=6.784E-4, N(O)=3.86893,
    N(SI)=1.36009
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=41.782601, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=6.503078, BP(CRISTOBALITE)=71.546701, BP(C_L)=0,
    BP(C_S)=20.051341, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   13 FROM STAGE    2
 H=-9.24576E5, P=1E5, N(C)=2.57094, N(N)=5.18E-4, N(O)=4.00556, N(SI)=2.24663
 DEGREES OF FREEDOM 0
T= 1.994519E+03
 BP(GAS)=57.417427, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.390387, BP(CRISTOBALITE)=63.260705, BP(C_L)=0,
    BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   13 FROM STAGE    3
 H=-7.374E5, P=1E5, N(C)=1.62655, N(N)=3.6E-4, N(O)=3.4643, N(SI)=2.69763
 DEGREES OF FREEDOM 0
T= 2.082731E+03
 BP(GAS)=63.654311, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.710227, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=52.365328, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   13 FROM STAGE    4
 H=79895.2, P=1E5, N(C)=0.865678, N(N)=2E-4, N(O)=1.7431, N(SI)=1.73723
 DEGREES OF FREEDOM 0
T= 2.721648E+03
 BP(GAS)=64.038962, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
    BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0, BP(DIAMOND)=0, BP(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=23.039395, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   14 FROM STAGE    1
 H=-1.00119E6, P=1E5, N(C)=3.26815, N(N)=6.784E-4, N(O)=3.86516,
    N(SI)=1.39888
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=41.977201, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=8.2717563, BP(CRISTOBALITE)=71.225272, BP(C_L)=0,
    BP(C_S)=18.915409, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   14 FROM STAGE    2
 H=-9.25814E5, P=1E5, N(C)=2.51969, N(N)=5.18E-4, N(O)=4.00932, N(SI)=2.2976
 DEGREES OF FREEDOM 0
T= 2.001975E+03
 BP(GAS)=56.899726, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.678344, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=64.366461, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   14 FROM STAGE    3
 H=-7.5344E5, P=1E5, N(C)=1.63225, N(N)=3.6E-4, N(O)=3.53706, N(SI)=2.7445
 DEGREES OF FREEDOM 0
T= 2.083146E+03
 BP(GAS)=65.078534, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.687761, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=53.512482, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   14 FROM STAGE    4
 H=65149.9, P=1E5, N(C)=0.865118, N(N)=2E-4, N(O)=1.78129, N(SI)=1.75576
 DEGREES OF FREEDOM 0
T= 2.649675E+03
 BP(GAS)=65.32767, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.875374, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
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 >>> DATA AT ITERATION   15 FROM STAGE    1
 H=-9.99863E5, P=1E5, N(C)=3.22232, N(N)=6.784E-4, N(O)=3.84582,
    N(SI)=1.42466
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=41.607103, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=9.4314277, BP(CRISTOBALITE)=71.039976, BP(C_L)=0,
    BP(C_S)=18.17504, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   15 FROM STAGE    2
 H=-9.28208E5, P=1E5, N(C)=2.49189, N(N)=5.18E-4, N(O)=4.03654, N(SI)=2.34977
 DEGREES OF FREEDOM 0
T= 2.011374E+03
 BP(GAS)=58.095637, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.727938, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=64.687648, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   15 FROM STAGE    3
 H=-7.66271E5, P=1E5, N(C)=1.63303, N(N)=3.6E-4, N(O)=3.5783, N(SI)=2.77058
 DEGREES OF FREEDOM 0
T= 2.083324E+03
 BP(GAS)=65.468306, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.724896, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=54.487322, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   15 FROM STAGE    4
 H=52616., P=1E5, N(C)=0.866044, N(N)=2E-4, N(O)=1.81374, N(SI)=1.77291
 DEGREES OF FREEDOM 0
T= 2.575864E+03
 BP(GAS)=66.468904, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.746114, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   16 FROM STAGE    1
 H=-1.00007E6, P=1E5, N(C)=3.19911, N(N)=6.784E-4, N(O)=3.86199,
    N(SI)=1.46355
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=42.375409, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=11.209864, BP(CRISTOBALITE)=70.703913, BP(C_L)=0,
    BP(C_S)=17.036615, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   16 FROM STAGE    2
 H=-9.28527E5, P=1E5, N(C)=2.44149, N(N)=5.18E-4, N(O)=4.03726, N(SI)=2.39893
 DEGREES OF FREEDOM 0
T= 2.020037E+03
 BP(GAS)=58.591617, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.771358, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=64.9352, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   16 FROM STAGE    3
 H=-7.76568E5, P=1E5, N(C)=1.63486, N(N)=3.6E-4, N(O)=3.6125, N(SI)=2.79319
 DEGREES OF FREEDOM 0
T= 2.083472E+03
 BP(GAS)=65.828605, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.789072, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=55.266805, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   16 FROM STAGE    4
 H=42605.3, P=1E5, N(C)=0.867644, N(N)=2E-4, N(O)=1.83968, N(SI)=1.78749
 DEGREES OF FREEDOM 0
T= 2.507706E+03
 BP(GAS)=67.422078, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.6366, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   17 FROM STAGE    1
 H=-9.99181E5, P=1E5, N(C)=3.15804, N(N)=6.784E-4, N(O)=3.8585, N(SI)=1.50085
 DEGREES OF FREEDOM 0
T= 1.785826E+03
 BP(GAS)=42.570551, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=12.913321, BP(CRISTOBALITE)=70.390442, BP(C_L)=0,
    BP(C_S)=15.949975, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   17 FROM STAGE    2
 H=-9.28656E5, P=1E5, N(C)=2.39393, N(N)=5.18E-4, N(O)=4.03732, N(SI)=2.4454
 DEGREES OF FREEDOM 0
T= 2.027376E+03
 BP(GAS)=59.074264, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.816728, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.141744, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   17 FROM STAGE    3
 H=-7.84668E5, P=1E5, N(C)=1.63727, N(N)=3.6E-4, N(O)=3.64014, N(SI)=2.81254
 DEGREES OF FREEDOM 0
T= 2.083598E+03
 BP(GAS)=66.144586, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.875519, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=55.878831, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   17 FROM STAGE    4
 H=34757.5, P=1E5, N(C)=0.8698, N(N)=2E-4, N(O)=1.86005, N(SI)=1.79983
 DEGREES OF FREEDOM 0
T= 2.447965E+03
 BP(GAS)=68.189741, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.56741, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   18 FROM STAGE    1
 H=-9.98331E5, P=1E5, N(C)=3.11923, N(N)=6.784E-4, N(O)=3.85516,
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    N(SI)=1.53616
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=42.75462, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=14.526164, BP(CRISTOBALITE)=70.093081, BP(C_L)=0,
    BP(C_S)=14.922322, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   18 FROM STAGE    2
 H=-9.28547E5, P=1E5, N(C)=2.34912, N(N)=5.18E-4, N(O)=4.03628, N(SI)=2.4885
 DEGREES OF FREEDOM 0
T= 2.033605E+03
 BP(GAS)=59.522044, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.858508, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.307946, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   18 FROM STAGE    3
 H=-7.9095E5, P=1E5, N(C)=1.64004, N(N)=3.6E-4, N(O)=3.66197, N(SI)=2.82819
 DEGREES OF FREEDOM 0
T= 2.083688E+03
 BP(GAS)=66.403735, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=34.965077, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=56.352236, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   18 FROM STAGE    4
 H=28693.2, P=1E5, N(C)=0.872034, N(N)=2E-4, N(O)=1.87581, N(SI)=1.80994
 DEGREES OF FREEDOM 0
T= 2.398231E+03
 BP(GAS)=68.793576, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.526539, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   19 FROM STAGE    1
 H=-9.97507E5, P=1E5, N(C)=3.08274, N(N)=6.784E-4, N(O)=3.8516, N(SI)=1.569
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=42.913712, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=16.026795, BP(CRISTOBALITE)=69.816123, BP(C_L)=0,
    BP(C_S)=13.966846, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   19 FROM STAGE    2
 H=-9.28273E5, P=1E5, N(C)=2.30776, N(N)=5.18E-4, N(O)=4.03429, N(SI)=2.52748
 DEGREES OF FREEDOM 0
T= 2.038832E+03
 BP(GAS)=59.919123, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.894909, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.440556, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   19 FROM STAGE    3
 H=-7.95775E5, P=1E5, N(C)=1.64273, N(N)=3.6E-4, N(O)=3.67899, N(SI)=2.84056
 DEGREES OF FREEDOM 0
T= 2.083751E+03
 BP(GAS)=66.611155, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.046899, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=56.715074, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   19 FROM STAGE    4
 H=24048.6, P=1E5, N(C)=0.874075, N(N)=2E-4, N(O)=1.88789, N(SI)=1.81802
 DEGREES OF FREEDOM 0
T= 2.358284E+03
 BP(GAS)=69.261142, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.503632, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   20 FROM STAGE    1
 H=-9.96727E5, P=1E5, N(C)=3.04912, N(N)=6.784E-4, N(O)=3.84782,
    N(SI)=1.59879
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.042147, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=17.38765, BP(CRISTOBALITE)=69.565063, BP(C_L)=0,
    BP(C_S)=13.10077, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   20 FROM STAGE    2
 H=-9.27909E5, P=1E5, N(C)=2.27042, N(N)=5.18E-4, N(O)=4.03169, N(SI)=2.56201
 DEGREES OF FREEDOM 0
T= 2.043175E+03
 BP(GAS)=60.262858, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.925514, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.546008, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   20 FROM STAGE    3
 H=-7.99465E5, P=1E5, N(C)=1.64513, N(N)=3.6E-4, N(O)=3.69216, N(SI)=2.85019
 DEGREES OF FREEDOM 0
T= 2.083795E+03
 BP(GAS)=66.774913, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.116375, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=56.991949, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   20 FROM STAGE    4
 H=20506.1, P=1E5, N(C)=0.875807, N(N)=2E-4, N(O)=1.89711, N(SI)=1.82436
 DEGREES OF FREEDOM 0
T= 2.326901E+03
 BP(GAS)=69.620223, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.490901, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   21 FROM STAGE    1
 H=-9.96006E5, P=1E5, N(C)=3.01883, N(N)=6.784E-4, N(O)=3.84399,
    N(SI)=1.62523
 DEGREES OF FREEDOM 0
T= 1.785827E+03
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 BP(GAS)=43.142841, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=18.595739, BP(CRISTOBALITE)=69.342397, BP(C_L)=0,
    BP(C_S)=12.332158, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   21 FROM STAGE    2
 H=-9.27508E5, P=1E5, N(C)=2.23735, N(N)=5.18E-4, N(O)=4.02883, N(SI)=2.59209
 DEGREES OF FREEDOM 0
T= 2.046761E+03
 BP(GAS)=60.555654, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.950682, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.629724, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   21 FROM STAGE    3
 H=-8.02281E5, P=1E5, N(C)=1.64714, N(N)=3.6E-4, N(O)=3.70232, N(SI)=2.85765
 DEGREES OF FREEDOM 0
T= 2.083827E+03
 BP(GAS)=66.903687, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.172897, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.202802, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   21 FROM STAGE    4
 H=17809.1, P=1E5, N(C)=0.877217, N(N)=2E-4, N(O)=1.90413, N(SI)=1.82928
 DEGREES OF FREEDOM 0
T= 2.302568E+03
 BP(GAS)=69.894827, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.483673, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   22 FROM STAGE    1
 H=-9.95358E5, P=1E5, N(C)=2.99203, N(N)=6.784E-4, N(O)=3.84029,
    N(SI)=1.64831
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.220493, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=19.65041, BP(CRISTOBALITE)=69.148216, BP(C_L)=0,
    BP(C_S)=11.6613, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   22 FROM STAGE    2
 H=-9.27105E5, P=1E5, N(C)=2.20849, N(N)=5.18E-4, N(O)=4.02593, N(SI)=2.61797
 DEGREES OF FREEDOM 0
T= 2.049708E+03
 BP(GAS)=60.802623, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.971114, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.696164, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   22 FROM STAGE    3
 H=-8.04427E5, P=1E5, N(C)=1.64878, N(N)=3.6E-4, N(O)=3.71015, N(SI)=2.86341
 DEGREES OF FREEDOM 0
T= 2.083850E+03
 BP(GAS)=67.00497, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.217744, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.363227, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   22 FROM STAGE    4
 H=15757.6, P=1E5, N(C)=0.878336, N(N)=2E-4, N(O)=1.90947, N(SI)=1.83307
 DEGREES OF FREEDOM 0
T= 2.283844E+03
 BP(GAS)=70.10435, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.479422, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   23 FROM STAGE    1
 H=-9.94784E5, P=1E5, N(C)=2.96867, N(N)=6.784E-4, N(O)=3.83684,
    N(SI)=1.66821
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.280015, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=20.559618, BP(CRISTOBALITE)=68.980974, BP(C_L)=0,
    BP(C_S)=11.083056, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   23 FROM STAGE    2
 H=-9.26721E5, P=1E5, N(C)=2.18361, N(N)=5.18E-4, N(O)=4.02315, N(SI)=2.64002
 DEGREES OF FREEDOM 0
T= 2.052127E+03
 BP(GAS)=61.00957, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=37.987587, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.748921, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   23 FROM STAGE    3
 H=-8.06062E5, P=1E5, N(C)=1.65008, N(N)=3.6E-4, N(O)=3.71618, N(SI)=2.86785
 DEGREES OF FREEDOM 0
T= 2.083867E+03
 BP(GAS)=67.084741, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.252804, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.485245, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   23 FROM STAGE    4
 H=14197.5, P=1E5, N(C)=0.87921, N(N)=2E-4, N(O)=1.91353, N(SI)=1.83597
 DEGREES OF FREEDOM 0
T= 2.269500E+03
 BP(GAS)=70.264029, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.476822, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   24 FROM STAGE    1
 H=-9.94284E5, P=1E5, N(C)=2.94854, N(N)=6.784E-4, N(O)=3.83371,
    N(SI)=1.68521
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.325565, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=21.335978, BP(CRISTOBALITE)=68.838273, BP(C_L)=0,
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    BP(C_S)=10.589354, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   24 FROM STAGE    2
 H=-9.26367E5, P=1E5, N(C)=2.16234, N(N)=5.18E-4, N(O)=4.02059, N(SI)=2.65869
 DEGREES OF FREEDOM 0
T= 2.054109E+03
 BP(GAS)=61.182135, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.000817, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.790851, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   24 FROM STAGE    3
 H=-8.07308E5, P=1E5, N(C)=1.65111, N(N)=3.6E-4, N(O)=3.72082, N(SI)=2.87127
 DEGREES OF FREEDOM 0
T= 2.083880E+03
 BP(GAS)=67.147677, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.279966, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.578049, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   24 FROM STAGE    4
 H=13011.1, P=1E5, N(C)=0.879887, N(N)=2E-4, N(O)=1.91662, N(SI)=1.8382
 DEGREES OF FREEDOM 0
T= 2.258538E+03
 BP(GAS)=70.385647, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.47517, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   25 FROM STAGE    1
 H=-9.93853E5, P=1E5, N(C)=2.93135, N(N)=6.784E-4, N(O)=3.83093,
    N(SI)=1.69961
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.360421, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=21.99399, BP(CRISTOBALITE)=68.717389, BP(C_L)=0,
    BP(C_S)=10.170944, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   25 FROM STAGE    2
 H=-9.26049E5, P=1E5, N(C)=2.1443, N(N)=5.18E-4, N(O)=4.01827, N(SI)=2.67439
 DEGREES OF FREEDOM 0
T= 2.055734E+03
 BP(GAS)=61.325485, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.011422, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.824206, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   25 FROM STAGE    3
 H=-8.08257E5, P=1E5, N(C)=1.65192, N(N)=3.6E-4, N(O)=3.7244, N(SI)=2.87392
 DEGREES OF FREEDOM 0
T= 2.083891E+03
 BP(GAS)=67.197436, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.300887, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.648623, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   25 FROM STAGE    4
 H=12109., P=1E5, N(C)=0.880409, N(N)=2E-4, N(O)=1.91897, N(SI)=1.83989
 DEGREES OF FREEDOM 0
T= 2.250176E+03
 BP(GAS)=70.478229, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.474083, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   26 FROM STAGE    1
 H=-9.93484E5, P=1E5, N(C)=2.91678, N(N)=6.784E-4, N(O)=3.82849,
    N(SI)=1.71175
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.38712, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=22.548387, BP(CRISTOBALITE)=68.615572, BP(C_L)=0,
    BP(C_S)=9.8184364, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   26 FROM STAGE    2
 H=-9.25767E5, P=1E5, N(C)=2.12908, N(N)=5.18E-4, N(O)=4.01622, N(SI)=2.68754
 DEGREES OF FREEDOM 0
T= 2.057064E+03
 BP(GAS)=61.444187, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.019917, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.850777, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   26 FROM STAGE    3
 H=-8.08981E5, P=1E5, N(C)=1.65255, N(N)=3.6E-4, N(O)=3.72717, N(SI)=2.87596
 DEGREES OF FREEDOM 0
T= 2.083898E+03
 BP(GAS)=67.236826, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.316946, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.702307, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   26 FROM STAGE    4
 H=11422.8, P=1E5, N(C)=0.88081, N(N)=2E-4, N(O)=1.92075, N(SI)=1.84119
 DEGREES OF FREEDOM 0
T= 2.243802E+03
 BP(GAS)=70.548707, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.473348, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   27 FROM STAGE    1
 H=-9.93171E5, P=1E5, N(C)=2.90449, N(N)=6.784E-4, N(O)=3.82638,
    N(SI)=1.72193
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.407586, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.013205, BP(CRISTOBALITE)=68.530222, BP(C_L)=0,
    BP(C_S)=9.5228976, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0,
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    BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   27 FROM STAGE    2
 H=-9.25521E5, P=1E5, N(C)=2.11631, N(N)=5.18E-4, N(O)=4.01443, N(SI)=2.69851
 DEGREES OF FREEDOM 0
T= 2.058154E+03
 BP(GAS)=61.54221, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.02672, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.871963, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   27 FROM STAGE    3
 H=-8.09533E5, P=1E5, N(C)=1.65304, N(N)=3.6E-4, N(O)=3.7293, N(SI)=2.87754
 DEGREES OF FREEDOM 0
T= 2.083905E+03
 BP(GAS)=67.268071, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.329238, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.74314, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   27 FROM STAGE    4
 H=10901., P=1E5, N(C)=0.881116, N(N)=2E-4, N(O)=1.92211, N(SI)=1.84217
 DEGREES OF FREEDOM 0
T= 2.238946E+03
 BP(GAS)=70.602342, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.472837, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   28 FROM STAGE    1
 H=-9.92907E5, P=1E5, N(C)=2.89418, N(N)=6.784E-4, N(O)=3.82457,
    N(SI)=1.73042
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.423288, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.401317, BP(CRISTOBALITE)=68.458958, BP(C_L)=0,
    BP(C_S)=9.2761342, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   28 FROM STAGE    2
 H=-9.25308E5, P=1E5, N(C)=2.10564, N(N)=5.18E-4, N(O)=4.01288, N(SI)=2.70763
 DEGREES OF FREEDOM 0
T= 2.059046E+03
 BP(GAS)=61.622972, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.03217, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.888876, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   28 FROM STAGE    3
 H=-8.09954E5, P=1E5, N(C)=1.65342, N(N)=3.6E-4, N(O)=3.73095, N(SI)=2.87876
 DEGREES OF FREEDOM 0
T= 2.083910E+03
 BP(GAS)=67.292882, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.338634, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.774205, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   28 FROM STAGE    4
 H=10504., P=1E5, N(C)=0.881351, N(N)=2E-4, N(O)=1.92315, N(SI)=1.84292
 DEGREES OF FREEDOM 0
T= 2.235248E+03
 BP(GAS)=70.643164, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.472476, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   29 FROM STAGE    1
 H=-9.92684E5, P=1E5, N(C)=2.88557, N(N)=6.784E-4, N(O)=3.82302,
    N(SI)=1.73749
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.435348, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.724248, BP(CRISTOBALITE)=68.399658, BP(C_L)=0,
    BP(C_S)=9.0708155, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   29 FROM STAGE    2
 H=-9.25125E5, P=1E5, N(C)=2.09675, N(N)=5.18E-4, N(O)=4.01156, N(SI)=2.71519
 DEGREES OF FREEDOM 0
T= 2.059777E+03
 BP(GAS)=61.689366, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.036539, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.902397, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   29 FROM STAGE    3
 H=-8.10275E5, P=1E5, N(C)=1.65372, N(N)=3.6E-4, N(O)=3.73223, N(SI)=2.8797
 DEGREES OF FREEDOM 0
T= 2.083913E+03
 BP(GAS)=67.312611, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.34581, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.797848, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   29 FROM STAGE    4
 H=10201.9, P=1E5, N(C)=0.88153, N(N)=2E-4, N(O)=1.92393, N(SI)=1.8435
 DEGREES OF FREEDOM 0
T= 2.232431E+03
 BP(GAS)=70.674243, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.472217, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   30 FROM STAGE    1
 H=-9.92498E5, P=1E5, N(C)=2.8784, N(N)=6.784E-4, N(O)=3.82172, N(SI)=1.74336
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.444613, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=23.992124, BP(CRISTOBALITE)=68.35046, BP(C_L)=0,
    BP(C_S)=8.9005013, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   30 FROM STAGE    2
 H=-9.2497E5, P=1E5, N(C)=2.08938, N(N)=5.18E-4, N(O)=4.01043, N(SI)=2.72144
```

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 DEGREES OF FREEDOM 0
T= 2.060375E+03
 BP(GAS)=61.743861, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.040041, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.913209, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   30 FROM STAGE    3
 H=-8.10519E5, P=1E5, N(C)=1.65395, N(N)=3.6E-4, N(O)=3.73322, N(SI)=2.88044
 DEGREES OF FREEDOM 0
T= 2.083916E+03
 BP(GAS)=67.328323, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.351284, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.815838, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   30 FROM STAGE    4
 H=9972.01, P=1E5, N(C)=0.881666, N(N)=2E-4, N(O)=1.92453, N(SI)=1.84393
 DEGREES OF FREEDOM 0
T= 2.230287E+03
 BP(GAS)=70.697896, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.472028, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   31 FROM STAGE    1
 H=-9.92343E5, P=1E5, N(C)=2.87245, N(N)=6.784E-4, N(O)=3.82061,
    N(SI)=1.74821
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.451746, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.213747, BP(CRISTOBALITE)=68.309747, BP(C_L)=0,
    BP(C_S)=8.7595943, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   31 FROM STAGE    2
 H=-9.24838E5, P=1E5, N(C)=2.08327, N(N)=5.18E-4, N(O)=4.00947, N(SI)=2.72659
 DEGREES OF FREEDOM 0
T= 2.060864E+03
 BP(GAS)=61.788518, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.042851, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.921864, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   31 FROM STAGE    3
 H=-8.10706E5, P=1E5, N(C)=1.65413, N(N)=3.6E-4, N(O)=3.73399, N(SI)=2.88101
 DEGREES OF FREEDOM 0
T= 2.083919E+03
 BP(GAS)=67.340846, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.355458, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.829529, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   31 FROM STAGE    4
 H=9797.11, P=1E5, N(C)=0.88177, N(N)=2E-4, N(O)=1.92499, N(SI)=1.84426
 DEGREES OF FREEDOM 0
T= 2.228654E+03
 BP(GAS)=70.715899, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471889, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   32 FROM STAGE    1
 H=-9.92213E5, P=1E5, N(C)=2.86752, N(N)=6.784E-4, N(O)=3.81969,
    N(SI)=1.75221
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.45724, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.396676, BP(CRISTOBALITE)=68.276134, BP(C_L)=0,
    BP(C_S)=8.6432873, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   32 FROM STAGE    2
 H=-9.24728E5, P=1E5, N(C)=2.07822, N(N)=5.18E-4, N(O)=4.00867, N(SI)=2.73083
 DEGREES OF FREEDOM 0
T= 2.061265E+03
 BP(GAS)=61.825057, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.045106, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.928798, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   32 FROM STAGE    3
 H=-8.10849E5, P=1E5, N(C)=1.65427, N(N)=3.6E-4, N(O)=3.73458, N(SI)=2.88145
 DEGREES OF FREEDOM 0
T= 2.083921E+03
 BP(GAS)=67.350838, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.358639, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.839947, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   32 FROM STAGE    4
 H=9664.01, P=1E5, N(C)=0.88185, N(N)=2E-4, N(O)=1.92533, N(SI)=1.84452
 DEGREES OF FREEDOM 0
T= 2.227412E+03
 BP(GAS)=70.729602, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471786, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   33 FROM STAGE    1
 H=-9.92106E5, P=1E5, N(C)=2.86345, N(N)=6.784E-4, N(O)=3.81892,
    N(SI)=1.75551
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.461476, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.547355, BP(CRISTOBALITE)=68.248438, BP(C_L)=0,
    BP(C_S)=8.5474842, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   33 FROM STAGE    2
 H=-9.24635E5, P=1E5, N(C)=2.07406, N(N)=5.18E-4, N(O)=4.008, N(SI)=2.73432
 DEGREES OF FREEDOM 0
T= 2.061592E+03
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 BP(GAS)=61.85492, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.046915, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.934354, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   33 FROM STAGE    3
 H=-8.10958E5, P=1E5, N(C)=1.65438, N(N)=3.6E-4, N(O)=3.73504, N(SI)=2.88179
 DEGREES OF FREEDOM 0
T= 2.083922E+03
 BP(GAS)=67.358817, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.361061, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.847874, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   33 FROM STAGE    4
 H=9562.77, P=1E5, N(C)=0.88191, N(N)=2E-4, N(O)=1.9256, N(SI)=1.84471
 DEGREES OF FREEDOM 0
T= 2.226466E+03
 BP(GAS)=70.740028, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471709, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   34 FROM STAGE    1
 H=-9.92018E5, P=1E5, N(C)=2.8601, N(N)=6.784E-4, N(O)=3.81828, N(SI)=1.75822
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.464746, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.671242, BP(CRISTOBALITE)=68.225658, BP(C_L)=0,
    BP(C_S)=8.4687148, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   34 FROM STAGE    2
 H=-9.24557E5, P=1E5, N(C)=2.07064, N(N)=5.18E-4, N(O)=4.00744, N(SI)=2.73718
 DEGREES OF FREEDOM 0
T= 2.061859E+03
 BP(GAS)=61.879293, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.048369, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.938812, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   34 FROM STAGE    3
 H=-8.11041E5, P=1E5, N(C)=1.65446, N(N)=3.6E-4, N(O)=3.7354, N(SI)=2.88206
 DEGREES OF FREEDOM 0
T= 2.083924E+03
 BP(GAS)=67.365192, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.362906, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.853906, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   34 FROM STAGE    4
 H=9485.72, P=1E5, N(C)=0.881956, N(N)=2E-4, N(O)=1.9258, N(SI)=1.84486
 DEGREES OF FREEDOM 0
T= 2.225747E+03
 BP(GAS)=70.747962, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471651, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   35 FROM STAGE    1
 H=-9.91944E5, P=1E5, N(C)=2.85734, N(N)=6.784E-4, N(O)=3.81775,
    N(SI)=1.76044
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.46727, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.77293, BP(CRISTOBALITE)=68.206954, BP(C_L)=0,
    BP(C_S)=8.4040588, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   35 FROM STAGE    2
 H=-9.24492E5, P=1E5, N(C)=2.06783, N(N)=5.18E-4, N(O)=4.00698, N(SI)=2.73952
 DEGREES OF FREEDOM 0
T= 2.062077E+03
 BP(GAS)=61.899163, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.049538, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.942391, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   35 FROM STAGE    3
 H=-8.11105E5, P=1E5, N(C)=1.65453, N(N)=3.6E-4, N(O)=3.73568, N(SI)=2.88226
 DEGREES OF FREEDOM 0
T= 2.083924E+03
 BP(GAS)=67.37029, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.364312, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.858499, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   35 FROM STAGE    4
 H=9427.07, P=1E5, N(C)=0.881991, N(N)=2E-4, N(O)=1.92595, N(SI)=1.84497
 DEGREES OF FREEDOM 0
T= 2.225199E+03
 BP(GAS)=70.754004, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471608, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   36 FROM STAGE    1
 H=-9.91884E5, P=1E5, N(C)=2.85508, N(N)=6.784E-4, N(O)=3.8173, N(SI)=1.76227
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.469218, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.856269, BP(CRISTOBALITE)=68.19162, BP(C_L)=0,
    BP(C_S)=8.3510689, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   36 FROM STAGE    2
 H=-9.24439E5, P=1E5, N(C)=2.06553, N(N)=5.18E-4, N(O)=4.00659, N(SI)=2.74144
 DEGREES OF FREEDOM 0
T= 2.062255E+03
 BP(GAS)=61.915351, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.050478, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.945263, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
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    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   36 FROM STAGE    3
 H=-8.11153E5, P=1E5, N(C)=1.65458, N(N)=3.6E-4, N(O)=3.7359, N(SI)=2.88242
 DEGREES OF FREEDOM 0
T= 2.083925E+03
 BP(GAS)=67.374369, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.365382, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.861994, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   36 FROM STAGE    4
 H=9382.43, P=1E5, N(C)=0.882018, N(N)=2E-4, N(O)=1.92607, N(SI)=1.84505
 DEGREES OF FREEDOM 0
T= 2.224782E+03
 BP(GAS)=70.758603, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471575, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   37 FROM STAGE    1
 H=-9.91834E5, P=1E5, N(C)=2.85322, N(N)=6.784E-4, N(O)=3.81694,
    N(SI)=1.76376
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.470726, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.924478, BP(CRISTOBALITE)=68.179065, BP(C_L)=0,
    BP(C_S)=8.3076978, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   37 FROM STAGE    2
 H=-9.24394E5, P=1E5, N(C)=2.06364, N(N)=5.18E-4, N(O)=4.00627, N(SI)=2.743
 DEGREES OF FREEDOM 0
T= 2.062401E+03
 BP(GAS)=61.928527, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.051232, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.947569, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   37 FROM STAGE    3
 H=-8.1119E5, P=1E5, N(C)=1.65462, N(N)=3.6E-4, N(O)=3.73607, N(SI)=2.88255
 DEGREES OF FREEDOM 0
T= 2.083926E+03
 BP(GAS)=67.377635, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.366197, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.864653, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   37 FROM STAGE    4
 H=9348.48, P=1E5, N(C)=0.882038, N(N)=2E-4, N(O)=1.92616, N(SI)=1.84512
 DEGREES OF FREEDOM 0
T= 2.224465E+03
 BP(GAS)=70.762101, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.47155, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   38 FROM STAGE    1
 H=-9.91794E5, P=1E5, N(C)=2.8517, N(N)=6.784E-4, N(O)=3.81664, N(SI)=1.76498
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.471895, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=24.980238, BP(CRISTOBALITE)=68.168798, BP(C_L)=0,
    BP(C_S)=8.2722425, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   38 FROM STAGE    2
 H=-9.24358E5, P=1E5, N(C)=2.0621, N(N)=5.18E-4, N(O)=4.00601, N(SI)=2.74428
 DEGREES OF FREEDOM 0
T= 2.062519E+03
 BP(GAS)=61.939241, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.05184, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.949422, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   38 FROM STAGE    3
 H=-8.11219E5, P=1E5, N(C)=1.65465, N(N)=3.6E-4, N(O)=3.7362, N(SI)=2.88265
 DEGREES OF FREEDOM 0
T= 2.083926E+03
 BP(GAS)=67.38025, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.366817, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.866677, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   38 FROM STAGE    4
 H=9322.64, P=1E5, N(C)=0.882053, N(N)=2E-4, N(O)=1.92622, N(SI)=1.84517
 DEGREES OF FREEDOM 0
T= 2.224223E+03
 BP(GAS)=70.764764, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471532, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   39 FROM STAGE    1
 H=-9.9176E5, P=1E5, N(C)=2.85046, N(N)=6.784E-4, N(O)=3.81639, N(SI)=1.76598
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.472799, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.025767, BP(CRISTOBALITE)=68.160411, BP(C_L)=0,
    BP(C_S)=8.243292, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   39 FROM STAGE    2
 H=-9.24327E5, P=1E5, N(C)=2.06084, N(N)=5.18E-4, N(O)=4.00579, N(SI)=2.74533
 DEGREES OF FREEDOM 0
T= 2.062616E+03
 BP(GAS)=61.947949, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.052328, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.95091, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   39 FROM STAGE    3
 H=-8.1124E5, P=1E5, N(C)=1.65467, N(N)=3.6E-4, N(O)=3.73631, N(SI)=2.88273
 DEGREES OF FREEDOM 0
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T= 2.083927E+03
 BP(GAS)=67.382345, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.367289, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.868216, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   39 FROM STAGE    4
 H=9303., P=1E5, N(C)=0.882065, N(N)=2E-4, N(O)=1.92628, N(SI)=1.8452
 DEGREES OF FREEDOM 0
T= 2.224040E+03
 BP(GAS)=70.766789, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471517, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   40 FROM STAGE    1
 H=-9.91733E5, P=1E5, N(C)=2.84944, N(N)=6.784E-4, N(O)=3.81619,
    N(SI)=1.76679
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.473502, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.062906, BP(CRISTOBALITE)=68.153568, BP(C_L)=0,
    BP(C_S)=8.2196764, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   40 FROM STAGE    2
 H=-9.24302E5, P=1E5, N(C)=2.05981, N(N)=5.18E-4, N(O)=4.00561, N(SI)=2.74618
 DEGREES OF FREEDOM 0
T= 2.062694E+03
 BP(GAS)=61.955019, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.052721, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.952106, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   40 FROM STAGE    3
 H=-8.11257E5, P=1E5, N(C)=1.65469, N(N)=3.6E-4, N(O)=3.73639, N(SI)=2.88279
 DEGREES OF FREEDOM 0
T= 2.083927E+03
 BP(GAS)=67.384024, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.367648, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.869388, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   40 FROM STAGE    4
 H=9288.04, P=1E5, N(C)=0.882074, N(N)=2E-4, N(O)=1.92631, N(SI)=1.84523
 DEGREES OF FREEDOM 0
T= 2.223900E+03
 BP(GAS)=70.76833, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471507, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   41 FROM STAGE    1
 H=-9.9171E5, P=1E5, N(C)=2.84862, N(N)=6.784E-4, N(O)=3.81602, N(SI)=1.76745
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.474045, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.09317, BP(CRISTOBALITE)=68.14799, BP(C_L)=0,
    BP(C_S)=8.2004316, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   41 FROM STAGE    2
 H=-9.24282E5, P=1E5, N(C)=2.05898, N(N)=5.18E-4, N(O)=4.00547, N(SI)=2.74687
 DEGREES OF FREEDOM 0
T= 2.062758E+03
 BP(GAS)=61.960758, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053037, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.953067, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   41 FROM STAGE    3
 H=-8.1127E5, P=1E5, N(C)=1.65471, N(N)=3.6E-4, N(O)=3.73645, N(SI)=2.88283
 DEGREES OF FREEDOM 0
T= 2.083927E+03
 BP(GAS)=67.385371, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.367921, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.870278, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   41 FROM STAGE    4
 H=9276.68, P=1E5, N(C)=0.882081, N(N)=2E-4, N(O)=1.92634, N(SI)=1.84525
 DEGREES OF FREEDOM 0
T= 2.223794E+03
 BP(GAS)=70.769502, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471498, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   42 FROM STAGE    1
 H=-9.91692E5, P=1E5, N(C)=2.84794, N(N)=6.784E-4, N(O)=3.81589,
    N(SI)=1.76799
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.474468, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.117812, BP(CRISTOBALITE)=68.143446, BP(C_L)=0,
    BP(C_S)=8.1847616, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   42 FROM STAGE    2
 H=-9.24265E5, P=1E5, N(C)=2.05829, N(N)=5.18E-4, N(O)=4.00535, N(SI)=2.74743
 DEGREES OF FREEDOM 0
T= 2.062810E+03
 BP(GAS)=61.965412, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053291, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.95384, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   42 FROM STAGE    3
 H=-8.11279E5, P=1E5, N(C)=1.65472, N(N)=3.6E-4, N(O)=3.7365, N(SI)=2.88287
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.38645, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368128, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
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    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.870955, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   42 FROM STAGE    4
 H=9268.04, P=1E5, N(C)=0.882086, N(N)=2E-4, N(O)=1.92637, N(SI)=1.84527
 DEGREES OF FREEDOM 0
T= 2.223713E+03
 BP(GAS)=70.770393, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471492, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   43 FROM STAGE    1
 H=-9.91677E5, P=1E5, N(C)=2.84739, N(N)=6.784E-4, N(O)=3.81578,
    N(SI)=1.76843
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.474797, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.13786, BP(CRISTOBALITE)=68.139748, BP(C_L)=0,
    BP(C_S)=8.1720129, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   43 FROM STAGE    2
 H=-9.24251E5, P=1E5, N(C)=2.05774, N(N)=5.18E-4, N(O)=4.00525, N(SI)=2.74789
 DEGREES OF FREEDOM 0
T= 2.062852E+03
 BP(GAS)=61.969186, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053495, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.954461, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   43 FROM STAGE    3
 H=-8.11287E5, P=1E5, N(C)=1.65473, N(N)=3.6E-4, N(O)=3.73654, N(SI)=2.8829
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.387316, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368286, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.87147, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   43 FROM STAGE    4
 H=9261.48, P=1E5, N(C)=0.88209, N(N)=2E-4, N(O)=1.92638, N(SI)=1.84528
 DEGREES OF FREEDOM 0
T= 2.223652E+03
 BP(GAS)=70.77107, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471487, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   44 FROM STAGE    1
 H=-9.91665E5, P=1E5, N(C)=2.84694, N(N)=6.784E-4, N(O)=3.81569,
    N(SI)=1.76878
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475052, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.154158, BP(CRISTOBALITE)=68.136742, BP(C_L)=0,
    BP(C_S)=8.1616487, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   44 FROM STAGE    2
 H=-9.2424E5, P=1E5, N(C)=2.05729, N(N)=5.18E-4, N(O)=4.00517, N(SI)=2.74826
 DEGREES OF FREEDOM 0
T= 2.062886E+03
 BP(GAS)=61.972243, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.05366, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.95496, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   44 FROM STAGE    3
 H=-8.11292E5, P=1E5, N(C)=1.65474, N(N)=3.6E-4, N(O)=3.73657, N(SI)=2.88292
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.38801, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368406, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.871861, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   44 FROM STAGE    4
 H=9256.48, P=1E5, N(C)=0.882093, N(N)=2E-4, N(O)=1.9264, N(SI)=1.84529
 DEGREES OF FREEDOM 0
T= 2.223605E+03
 BP(GAS)=70.771585, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471484, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   45 FROM STAGE    1
 H=-9.91655E5, P=1E5, N(C)=2.84658, N(N)=6.784E-4, N(O)=3.81561,
    N(SI)=1.76907
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475251, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.167399, BP(CRISTOBALITE)=68.134298, BP(C_L)=0,
    BP(C_S)=8.1532287, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   45 FROM STAGE    2
 H=-9.24231E5, P=1E5, N(C)=2.05692, N(N)=5.18E-4, N(O)=4.0051, N(SI)=2.74856
 DEGREES OF FREEDOM 0
T= 2.062914E+03
 BP(GAS)=61.974718, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053792, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.955362, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   45 FROM STAGE    3
 H=-8.11297E5, P=1E5, N(C)=1.65474, N(N)=3.6E-4, N(O)=3.73659, N(SI)=2.88294
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.388568, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368497, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.872159, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_QUARTZ_S2)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
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    BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
 >>> DATA AT ITERATION   45 FROM STAGE    4
 H=9252.69, P=1E5, N(C)=0.882095, N(N)=2E-4, N(O)=1.92641, N(SI)=1.8453
 DEGREES OF FREEDOM 0
T= 2.223570E+03
 BP(GAS)=70.771976, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471481, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   46 FROM STAGE    1
 H=-9.91647E5, P=1E5, N(C)=2.84628, N(N)=6.784E-4, N(O)=3.81555,
    N(SI)=1.76931
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475405, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.178148, BP(CRISTOBALITE)=68.132314, BP(C_L)=0,
    BP(C_S)=8.1463928, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   46 FROM STAGE    2
 H=-9.24223E5, P=1E5, N(C)=2.05662, N(N)=5.18E-4, N(O)=4.00505, N(SI)=2.7488
 DEGREES OF FREEDOM 0
T= 2.062937E+03
 BP(GAS)=61.976723, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053899, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.955685, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   46 FROM STAGE    3
 H=-8.113E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73661, N(SI)=2.88295
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.389015, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368566, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.872385, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   46 FROM STAGE    4
 H=9249.81, P=1E5, N(C)=0.882097, N(N)=2E-4, N(O)=1.92641, N(SI)=1.8453
 DEGREES OF FREEDOM 0
T= 2.223543E+03
 BP(GAS)=70.772274, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471479, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   47 FROM STAGE    1
 H=-9.9164E5, P=1E5, N(C)=2.84604, N(N)=6.784E-4, N(O)=3.8155, N(SI)=1.7695
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475526, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.18687, BP(CRISTOBALITE)=68.130703, BP(C_L)=0,
    BP(C_S)=8.140846, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   47 FROM STAGE    2
 H=-9.24217E5, P=1E5, N(C)=2.05638, N(N)=5.18E-4, N(O)=4.00501, N(SI)=2.749
 DEGREES OF FREEDOM 0
T= 2.062955E+03
 BP(GAS)=61.978345, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.053985, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.955944, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   47 FROM STAGE    3
 H=-8.11303E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73663, N(SI)=2.88296
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.389374, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368619, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.872556, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   47 FROM STAGE    4
 H=9247.62, P=1E5, N(C)=0.882098, N(N)=2E-4, N(O)=1.92642, N(SI)=1.84531
 DEGREES OF FREEDOM 0
T= 2.223522E+03
 BP(GAS)=70.772499, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471478, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   48 FROM STAGE    1
 H=-9.91635E5, P=1E5, N(C)=2.84585, N(N)=6.784E-4, N(O)=3.81546,
    N(SI)=1.76965
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.47562, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.193943, BP(CRISTOBALITE)=68.129397, BP(C_L)=0,
    BP(C_S)=8.1363478, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   48 FROM STAGE    2
 H=-9.24212E5, P=1E5, N(C)=2.05618, N(N)=5.18E-4, N(O)=4.00497, N(SI)=2.74916
 DEGREES OF FREEDOM 0
T= 2.062970E+03
 BP(GAS)=61.979657, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.054054, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.956153, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   48 FROM STAGE    3
 H=-8.11304E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73664, N(SI)=2.88297
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.389662, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368659, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.872687, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   48 FROM STAGE    4
 H=9245.96, P=1E5, N(C)=0.882099, N(N)=2E-4, N(O)=1.92642, N(SI)=1.84531
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 DEGREES OF FREEDOM 0
T= 2.223507E+03
 BP(GAS)=70.772671, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471476, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   49 FROM STAGE    1
 H=-9.91631E5, P=1E5, N(C)=2.84569, N(N)=6.784E-4, N(O)=3.81543,
    N(SI)=1.76978
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475694, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.199676, BP(CRISTOBALITE)=68.128338, BP(C_L)=0,
    BP(C_S)=8.1327019, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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   49 FROM STAGE    2
 H=-9.24208E5, P=1E5, N(C)=2.05603, N(N)=5.18E-4, N(O)=4.00494, N(SI)=2.74929
 DEGREES OF FREEDOM 0
T= 2.062982E+03
 BP(GAS)=61.980717, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.054109, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.956321, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   49 FROM STAGE    3
 H=-8.11306E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73665, N(SI)=2.88298
 DEGREES OF FREEDOM 0
T= 2.083928E+03
 BP(GAS)=67.389893, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368689, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.872786, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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   49 FROM STAGE    4
 H=9244.7, P=1E5, N(C)=0.8821, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84531
 DEGREES OF FREEDOM 0
T= 2.223495E+03
 BP(GAS)=70.772801, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471475, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
 >>> DATA AT ITERATION   50 FROM STAGE    1
 H=-9.91627E5, P=1E5, N(C)=2.84556, N(N)=6.784E-4, N(O)=3.8154, N(SI)=1.76988
 DEGREES OF FREEDOM 0
T= 1.785827E+03
 BP(GAS)=43.475751, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=25.204321, BP(CRISTOBALITE)=68.12748, BP(C_L)=0,
    BP(C_S)=8.1297481, BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=0,
    BP(O2SI1_QUARTZ)=0, BP(O2SI1_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)=61.981575, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=38.054154, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=65.956456, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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)=67.390079, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
    BP(C1SI1_BETA)=35.368712, BP(CRISTOBALITE)=0, BP(C_L)=0, BP(C_S)=0,
    BP(DIAMOND)=0, BP(N4SI3_S)=0, BP(O2SI1_L)=57.872861, BP(O2SI1_QUARTZ)=0,
    BP(O2SI1_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=9243.75, P=1E5, N(C)=0.882101, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84532
 DEGREES OF FREEDOM 0
T= 2.223486E+03
 BP(GAS)=70.7729, 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(N4SI3_S)=0,
    BP(O2SI1_L)=0, BP(O2SI1_QUARTZ)=0, BP(O2SI1_QUARTZ_S2)=0,
    BP(SI_L)=22.471475, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
    BP(TRIDYMITE_S3)=0
 ================================
REACTOR: @@ Use POLY-3 to list the constitution in each segment
REACTOR: GO P-3
POLY: L-E
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =  1004, label A0  , database: SSUB6

 Conditions:
 H=9243.75, P=1E5, N(C)=0.882101, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84532
 DEGREES OF FREEDOM 0

 Temperature   2223.49 K (  1950.34 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  9.24375E+03,  Volume  3.56321E-01

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        8.8210E-01  1.1363E-01 5.0908E-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 1.5639E-03 -1.1944E+05 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 3.8539E+00, Mass 7.0773E+01, Volume fraction 1.0000E+00  Mass fractions:
 O   4.35491E-01  SI  4.14766E-01  C   1.49703E-01  N   3.95829E-05
 Constitution:
 O1SI1  5.41812E-01  C1O2   2.03423E-05  C      2.35264E-10  O2     9.78900E-14
 C1O1   4.57645E-01  O2SI1  1.70445E-06  N1O1   7.37247E-11
 SI     4.69580E-04  C1SI1  3.44146E-09  C3     4.10890E-12
 N2     5.18835E-05  O      9.79789E-10  C2     3.46788E-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: @@ This equilibrium is valid for the fourth segment. Note it is

POLY: @@ identified with number 1004. The other have numbers 1001,
POLY: @@ 1002 and 1003.
POLY:
POLY: go sys
SYS: set-inter
SYS:
```

tcex25

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex25\tcex25.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Simulating the refinement of steel
SYS:
SYS: @@ This example is based on a typical steel refining process.
SYS: @@ Raw iron used to produce steel usually has high carbon and
SYS: @@ silicon content, which is why oxygen is blown into the
SYS: @@ furnace to burn off carbon. Lime (CaO) is added to form a
SYS: @@ slag with silica, and the slag can be removed. Alloying
SYS: @@ elements, such as Mn, Ni, Cr and V are added to produce
SYS: @@ the desired steel. Since the reaction between O and C
SYS: @@ increases the temperature, scrap iron is added to keep
SYS: @@ the temperature constant (it is assumed the furnace is
SYS: @@ isolated and no heat is lost to the environment).
SYS:
SYS: @@ This example simulates blowing oxygen into a liquid steel
SYS: @@ of  one metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and
SYS: @@ 1 w/o Mn. 100 moles of CaO (equivalent to 5.6 kg) is added.
SYS: @@ Keeping the enthalpy constant is the way to simulate the
SYS: @@ isolation of the furnace. The oxygen reacts with carbon
SYS: @@ and increases the temperature. After blowing a certain
SYS: @@ amount of oxygen, scrap iron is added to keep the
SYS: @@ temperature constant.
SYS:
SYS: @@ Note that a SLAG database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex25,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: @@ In this example we use data from the SLAG database
TDB_TCFE10: sw slag4
   ... the command in full is SWITCH_DATABASE
 Current database: Fe-containing Slag  v4.1

 FE                      O  DEFINED
 FEOLIQ  REJECTED
TDB_SLAG4: d-sys ca si mn c
   ... the command in full is DEFINE_SYSTEM
 CA                      SI                      MN
 C  DEFINED
TDB_SLAG4: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 GAS:G       :C1O1 C1O2 O2:
  > The gaseous mixture is handled by the ideal gas model
 FE_LIQUID:L :C CA FE MN O SI:
  > Fe-rich liquid phase (dilute solution for other elements)
 SLAG:L      :A0_01_C00C04_12_SIO2 A0_01_C00C10_23_FE2O3 A0_01_C00C16_11_FEO
  A0_01_C00C22_11_MNO A0_01_C00C27_11_CAO A0_01_C04C10_SIFE
  A0_01_C04C16_SIFE A0_01_C04C22_SIMN A0_01_C04C27_SICA A0_01_C10C16_FEFE
  A0_01_C10C22_FEMN A0_01_C10C27_FECA A0_01_C16C22_FEMN A0_01_C16C27_FECA
  A0_01_C22C27_MNCA:
  > Slag phase handled by Kapoor-Frohberg-Gaye Quasichemical Cell Model
 CAO         :CAO:
  > This is pure CaO_Lime phase [CaO]
 FEO         :FEO:
  > This is pure FeO_Wustite phase [FeO]
 FE2O3       :FE2O3:
  > This is pure Fe2O3_Hematite phase [Fe2O3]
 FE3O4       :FE3O4:
  > This is pure Fe3O4_Magnetite phase [Fe3O4]
 MNO         :MNO:
  > This is pure MnO_Manganosite phase [MnO]
 SIO2        :SIO2:
  > This is tridymite or cristobalite (in the SLAG-stable T range)
 CA3O3_SIO2  :CAO:SIO2:
  > This is pure Ca3SiO5 phase [3CaO-SiO2]
 CA2O2_SIO2  :CAO:SIO2:
  > This is pure Ca2SiO4 phase [2CaO-SiO2]
 CA3O3_SI2O4 :CAO:SIO2:
  > This is pure Ca3Si2O7 phase [3CaO-2SiO2]
 CAO_SIO2    :CAO:SIO2:
  > This is pure CaSiO3 phase [CaO-SiO2]
 FE2O2_SIO2  :FEO:SIO2:
  > This is pure Fe2SiO4 phase [2FeO-SiO2]
 MN2O2_SIO2  :MNO:SIO2:
  > This is pure Mn2SiO4 phase [2MnO-SiO2]
 MNO_SIO2    :MNO:SIO2:
  > This is pure MnSiO3 phase [MnO-SiO2]
 GRAPHITE    :C:
TDB_SLAG4: get
   ... the command in full is GET_DATA
15:21:14,441 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
```

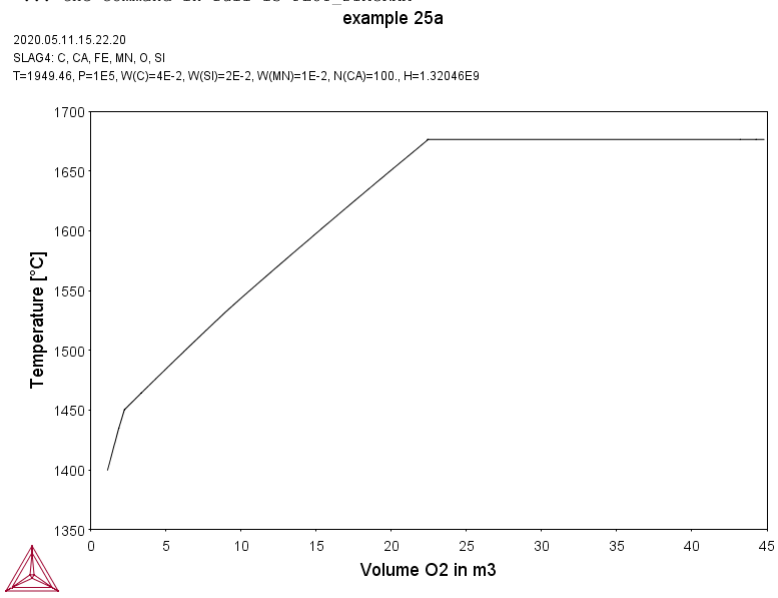
```
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set SLAG#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'SLAG2 (2006): TCS Fe-Containing Slag Database, V2.3, owned and provided
      by Thermo-Calc Software.'
  'L Kjellqvist (2013), unpublished work; Fe3O4 stability'
  'TCMP2 (2009): TCS Materials Processing Database, V2.5, owned and provided
      by Thermo-Calc Software.'
 -OK-
15:21:17,336 WARN  The handling of the fraction limits command is not yet supported in GES6.
15:21:17,349 WARN  The handling of the default stable command is not yet supported in GES6.
TDB_SLAG4: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ Assume we have one ton (1e6 gram) liquid steel with a

POLY: @@ composition set of 4 w/o C, 2 w/o Si and 1 w/o Mn.
POLY: 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: 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:Hit RETURN to continue
POLY: @@ To remove Si, add a small amount of top slag consisting of
POLY: @@ pure lime (CaO), 5.6 kg equivalent to 100 moles of CaO
POLY: s-i-a n(cao)=100
   ... the command in full is SET_INPUT_AMOUNTS
POLY: 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:Hit RETURN to continue
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          4030 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       2 s, total time     2  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG4

 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:Hit RETURN to continue
POLY: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 CAO                     ENTERED      0.000000E+00    1.999545E+02
 CA3O3_SIO2              ENTERED      0.000000E+00    1.231298E-02
 FE_LIQUID               ENTERED      0.000000E+00    2.247397E+04
 CA2O2_SIO2              ENTERED     -1.474286E-01    0.000000E+00
 GRAPHITE                ENTERED     -1.870471E-01    0.000000E+00
 SLAG#1                  ENTERED     -3.283110E-01    0.000000E+00
 SLAG#2                  ENTERED     -3.283110E-01    0.000000E+00
 CA3O3_SI2O4             ENTERED     -4.942106E-01    0.000000E+00
 CAO_SIO2                ENTERED     -1.019253E+00    0.000000E+00
 GAS                     ENTERED     -2.389247E+00    0.000000E+00
 SIO2                    ENTERED     -3.679778E+00    0.000000E+00
 MNO_SIO2                ENTERED     -3.699744E+00    0.000000E+00
 MN2O2_SIO2              ENTERED     -3.772584E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -4.566408E+00
 MNO FE2O2_SIO2 FEO FE3O4 FE2O3
POLY:Hit RETURN to continue
POLY: @@ The steel bath is insulated so no heat disappears while
POLY: @@ blowing oxygen. This means that the enthalpy of the system
POLY: @@ is constant and the temperature may increase. Set these
POLY: @@ conditions
POLY:
POLY: s-c h
   ... the command in full is SET_CONDITION
Value /1.32045762E+09/:
POLY: s-c t=none
   ... the command in full is SET_CONDITION
POLY: 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:Hit RETURN to continue
POLY: @@ When calculated, it should get exactly the same temperature.
POLY: 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   2 SECONDS
POLY: sh t
   ... the command in full is SHOW_VALUE
 T=1673.
POLY: @@ The same equilibrium calculated with different conditions
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG4

 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:Hit RETURN to continue
POLY: @@ Now set the oxygen content as independent variable and blow
POLY: @@ up to 2000 moles of O (i.e. 1000 moles of O2 i.e. 22.4 m3)
POLY:
POLY: 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: save tcex25 y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    100.000
...OK

 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  2.02167E+02
 Calculated     3 equilibria

 Phase Region from    202.167     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  1.00000E+03 .... OK
 Global test at  2.00000E+03 .... OK
 Terminating at    2000.00
 Calculated    21 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex25\tcex25.POLY3
POLY: @@ Sometimes error 1614 dispalys. It means all conditions
POLY: @@ are not fullfilled. Try to start with more oxygen.
POLY:
POLY: read tcex25
   ... the command in full is READ_WORKSPACES
POLY:
POLY: s-c n(o)
   ... the command in full is SET_CONDITION
Value /100/: 200
```

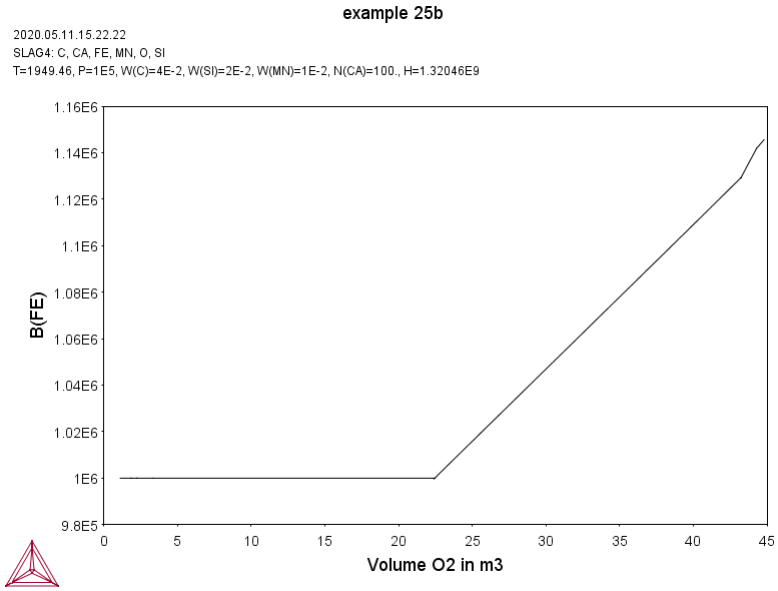
```
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          4030 grid points in             0 s
    94 ITS,  CPU TIME USED   2 SECONDS
POLY: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG4

 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 5.5488E-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:Hit RETURN to continue
POLY: @@ if still trouble, add that gas should be stable
POLY: @@ (gas dissolves all) by increasing oxygen content
POLY: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 CA3O3_SIO2              ENTERED      0.000000E+00    1.408525E+00
 CA2O2_SIO2              ENTERED      0.000000E+00    3.483550E+02
 FE_LIQUID               ENTERED      0.000000E+00    2.243144E+04
 SLAG#1                  ENTERED     -1.466609E-01    0.000000E+00
 SLAG#2                  ENTERED     -1.466609E-01    0.000000E+00
 CA3O3_SI2O4             ENTERED     -2.500340E-01    0.000000E+00
 GRAPHITE                ENTERED     -2.698781E-01    0.000000E+00
 CAO                     ENTERED     -4.788199E-01    0.000000E+00
 CAO_SIO2                ENTERED     -6.202161E-01    0.000000E+00
 GAS                     ENTERED     -1.307472E+00    0.000000E+00
 SIO2                    ENTERED     -2.641471E+00    0.000000E+00
 MNO_SIO2                ENTERED     -2.764554E+00    0.000000E+00
 MN2O2_SIO2              ENTERED     -2.883913E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -3.757734E+00
 MNO FE2O2_SIO2 FEO FE3O4 FE2O3
POLY: c-st p gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of mole formula units /0/: 1
POLY: s-c n(o)=300
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          4030 grid points in             0 s
    39 ITS,  CPU TIME USED   1 SECONDS
POLY: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SLAG4

 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 -2.42506E+09,  Enthalpy  1.32046E+09,  Volume  1.41371E+01

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.6125E+03  4.0000E-02 5.9861E-02 -4.0675E+04 SER
 CA                      1.0000E+02  3.6947E-03 1.1355E-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 4.1968E-06 -1.7886E+05 SER
 O                       3.0000E+02  4.4248E-03 1.1813E-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 1.9574E+02, Mass 2.7414E+03, Volume fraction 1.0000E+00  Mass fractions:
 O   5.71227E-01  SI  0.00000E+00  FE  0.00000E+00
 C   4.28773E-01  MN  0.00000E+00  CA  0.00000E+00
 Constitution:
 C1O1  9.99844E-01  C1O2  1.55552E-04  O2    2.65151E-16

 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  9.31631E-01  SI  1.89033E-02  O   3.16146E-05
 C   3.93280E-02  MN  1.01058E-02  CA  8.34231E-13

 CA2O2_SIO2                  Status ENTERED     Driving force  0.0000E+00
 Moles 3.5000E+02, Mass 8.6119E+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:Hit RETURN to continue
POLY: 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: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    300.000
...OK

 Phase Region from    300.000     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  1.10000E+03 .... OK
 Terminating at    2000.00
 Calculated    20 equilibria

 Phase Region from    300.000     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global check of removing phase at  2.02167E+02
 Calculated     3 equilibria

 Phase Region from    202.167     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: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex25\tcex25.POLY3
POLY:
POLY: @@ The calculation up to 2000 moles is saved to file.
POLY: @@ Now change the conditions and start adding scrap to
POLY: @@ keep the temperature constant. However, the current
POLY: @@ equilibrium is at 100 moles of O so we must first
POLY: @@ make an interactive calculation at 2000 moles.
POLY:
POLY: read tcex25
   ... the command in full is READ_WORKSPACES
POLY:
POLY: s-c n(o)
   ... the command in full is SET_CONDITION
Value /300/: 2005
POLY: @@ Choose the value a little bigger than 2000 moles or
POLY: @@ the upper limit of the previous calculation coincides
POLY: @@ with the lower limit of this calculation and that
POLY: @@ causes trouble
POLY:
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          4030 grid points in             0 s
    24 ITS,  CPU TIME USED   1 SECONDS
POLY: sh t
   ... the command in full is SHOW_VALUE
 T=1949.4617
POLY: @@ We now want to keep the temperature constant by
POLY: @@ adding scrap.
POLY: @@ Set the temperature as condition
POLY: s-c t
   ... the command in full is SET_CONDITION
Value /1949.461709/:
POLY:
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=1949.46, 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:Hit RETURN to continue
POLY: @@ There are too many conditions. Assuming the scrap
POLY: @@ is pure iron we can just release the condition on
POLY: @@ the amount of Fe.
POLY:
POLY: s-c b(fe)
   ... the command in full is SET_CONDITION
Value /1000000/: none
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=1949.46, 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:Hit RETURN to continue
POLY: @@ It is rather special to have both enthalpy
POLY: @@ and temperature set as conditions.
POLY: @@ We must change the axis limits
POLY: 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
```

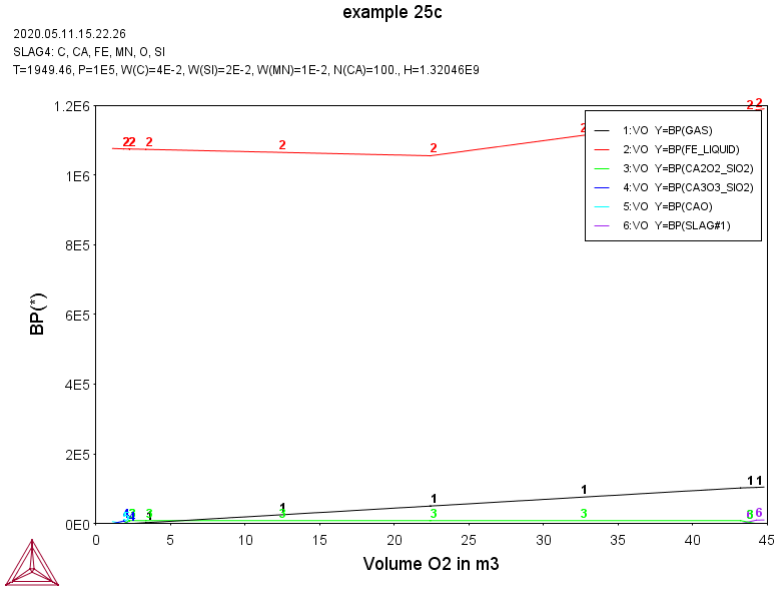
```
POLY: @@ We must not give a Save command now as that would
POLY: @@ destroy the results from the previous Step command.
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    2005.00
...OK

 Phase Region from    2005.00     for:
     GAS
     FE_LIQUID
     CA2O2_SIO2
 Global test at  2.80500E+03 .... OK
 Global test at  3.80500E+03 .... OK
 Global check of adding phase at  3.85963E+03
 Calculated    21 equilibria

 Phase Region from    3859.63     for:
     GAS
     FE_LIQUID
     SLAG#1
     CA2O2_SIO2
 Global check of removing phase at  3.95422E+03
 Calculated     4 equilibria

 Phase Region from    3954.22     for:
     GAS
     FE_LIQUID
     SLAG#1
 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: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex25\tcex25.POLY3
POLY: @@ We now plot the combined results
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: @@ Use volume of added O2 as independent axis,
POST: @@ 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:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



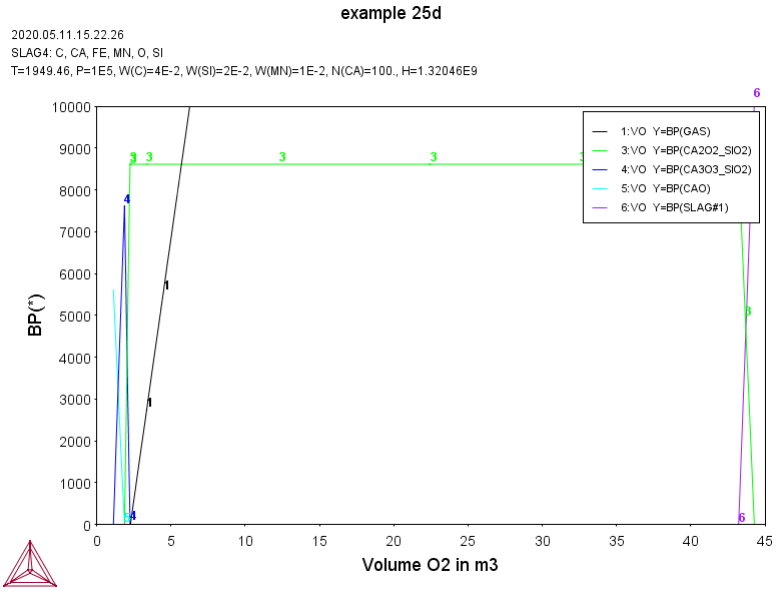

```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the amount of Fe (in grams)
POST: s-d-a y b(fe)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 25b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



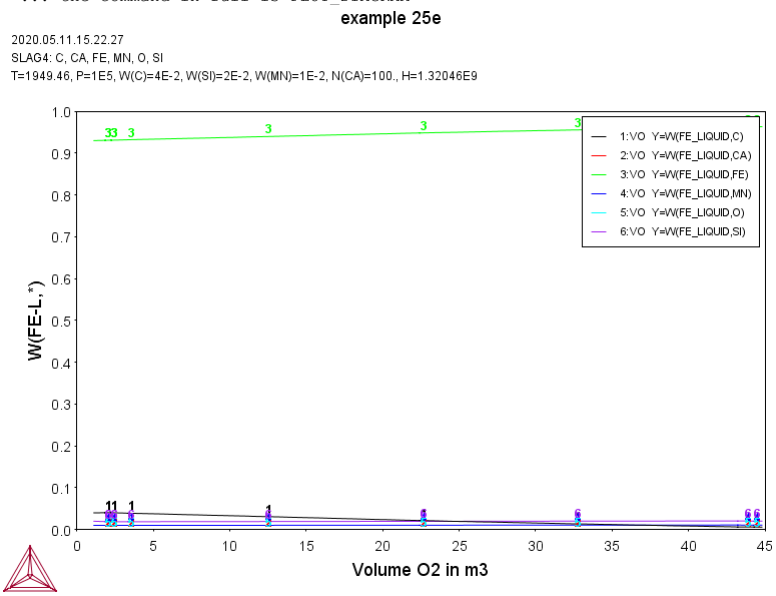

```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the mass of all phases
POST: s-d-a y bp(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: set-lab D
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 25c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



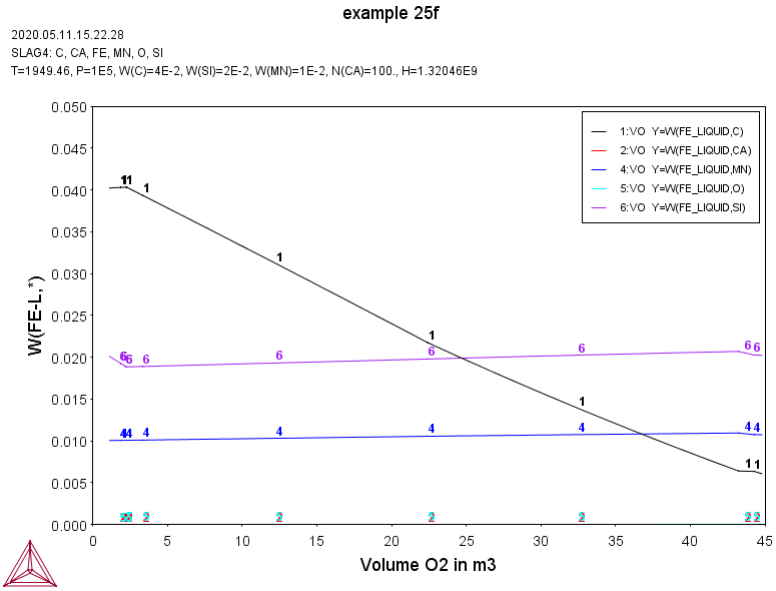

```
POST:
POST:Hit RETURN to continue
POST: @@ Scale up the slag amount. Liquid slags come
POST: @@ at the end only.
POST: s-s y n 0 10000
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 25d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



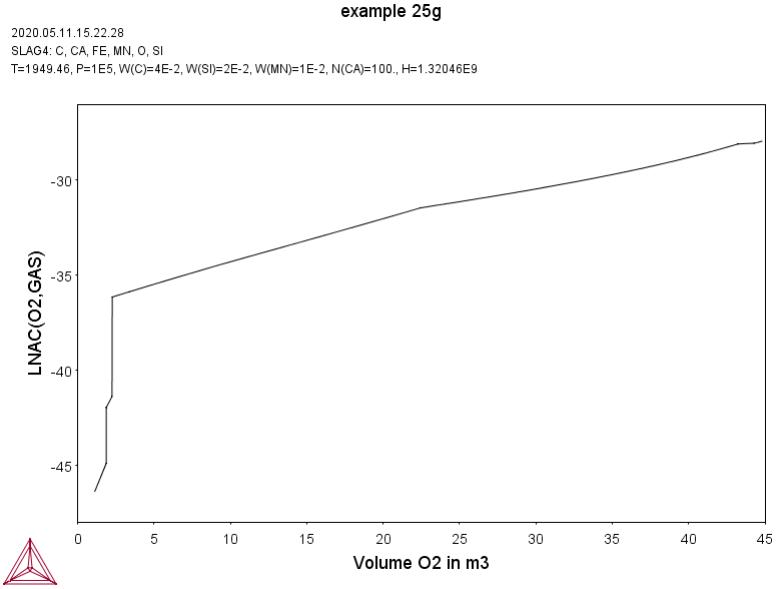

```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot the reason for this: the steel composition
POST: s-d-a y w(fe-l,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: set-title example 25e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



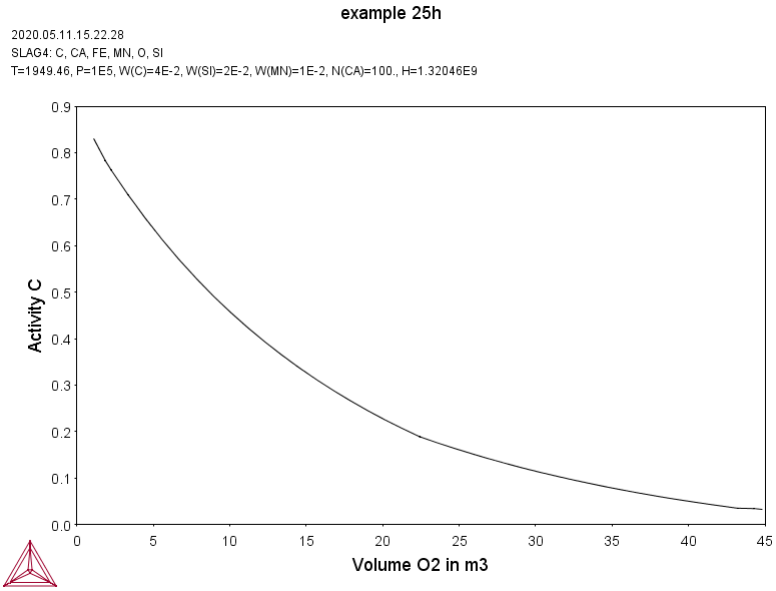

```
POST:
POST:Hit RETURN to continue
POST: @@ Scale up the diagram to get the important part
POST: s-s y n 0 .05
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 25f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Finally plot the oxygen partial pressure and
POST: @@ carbon activity. For the oxygen plot LN(activity)
POST: s-d-a y lnac(o2,gas)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-lab none
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 25g
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST:
POST:
POST: @@ For carbon do not forget to Set Reference State
POST: set-ref-state c gra * 1e5
   ... the command in full is SET_REFERENCE_STATE
 You should set-diagram-axis for the activity/potential after this!
POST: s-d-a y ac c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 25h
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST:
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex26

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex26\tcex26.TCM.test"
SYS: set-echo
SYS:
SYS: @@ The As-Ga phase diagram: Plotting the partial pressures
SYS: @@ of a gas species
SYS:
SYS: @@ This is an example of plotting the partial pressures
SYS: @@ of a gas species along the solubility lines in the As-Ga
SYS: @@ phase diagram. The calculation makes it possible to monitor
SYS: @@ the input gases to a process of depositing solid As-Ga.
SYS:
SYS: set-log ex26,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: @@ The data is taken from the special III-V database
TDB_TCFE10:
TDB_TCFE10: sw
   ... the command in full is SWITCH_DATABASE
 Use one of these databases

 TCFE10  =  Steels/Fe-Alloys  v10.1
 TCFE9   =  Steels/Fe-Alloys  v9.2
 TCFE8   =  Steels/Fe-Alloys  v8.1
 TCFE7   =  Steels/Fe-Alloys  v7.0
 TCFE6   =  Steels/Fe-Alloys  v6.2
 TCFE5   =  Steels/Fe-Alloys  v5.0
 TCFE4   =  Steels/Fe-Alloys  v4.1
 TCFE3   =  Steels/Fe-Alloys  v3.1
 TCFE2   =  Steels/Fe-Alloys  v2.1
 TCFE1   =  Steels/Fe-Alloys  v1.0
 FROST1  =  FROST database v1.2
 FEDAT   =  TCS/TT Steels Database v1.0
 TCNI10  =  Ni-Alloys  v10.0
 TCNI9   =  Ni-Alloys  v9.1
 TCNI8   =  Ni-Alloys  v8.2
 TCNI7   =  Ni-Alloys  v7.2
 TCNI6   =  Ni-Alloys  v6.1
 TCNI5   =  Ni-Alloys  v5.1
 TCNI4   =  Ni-Alloys  v4.0
 TCNI1   =  Ni-Alloys  v1.3
 TCAL6   =  Al-Alloys  v6.0
 TCAL5   =  Al-Alloys  v5.1
 TCAL4   =  Al-Alloys  v4.0
 TCAL3   =  Al-Alloys  v3.0
 TCAL2   =  Al-Alloys  v2.1
 TCAL1   =  Al-Alloys  v1.2
 TCMG5   =  Mg-Alloys  v5.1
 TCMG4   =  Mg-Alloys  v4.0
 TCMG3   =  Mg-Alloys  v3.0
 TCMG2   =  Mg-Alloys  v2.0
 TCMG1   =  Mg-Alloys  v1.1
 TCTI2   =  Ti-Alloys  v2.2
 TCTI1   =  Ti-Alloys  v1.0
 TCCU3   =  Cu-Alloys  v3.1
 TCCU2   =  Cu-Alloys  v2.0
 TCCU1   =  Cu-Alloys  v1.0
 TCCC1   =  Cemented carbide  v1.0
 TCHEA4  =  High Entropy Alloy  v4.1
 TCHEA3  =  High Entropy Alloy  v3.1
 TCHEA2  =  High Entropy Alloy  v2.1.1
 TCHEA1  =  High Entropy Alloy  v1.0
 SSOL7   =  SGTE Alloy Solutions Database v7.0
 SSOL6   =  SGTE Alloy Solutions Database v6.0
 SSOL5   =  SGTE Alloy Solutions Database v5.0
 SSOL4   =  SGTE Alloy Solutions Database v4.9g
 SSOL2   =  SGTE Alloy Solutions Database v2.1
 SSUB6   =  SGTE Substances Database v6.0
 SSUB5   =  SGTE Substances Database v5.2
 SSUB4   =  SGTE Substances Database v4.1
 SSUB3   =  SGTE Substances Database v3.3
 SSUB2   =  SGTE Substances Database v2.2
 SNOB3   =  SGTE Noble Metal Alloys Database v3.1
 STBC2   =  SGTE Thermal Barrier Coating TDB v2.2
 STBC1   =  SGTE Thermal Barrier Coating TDB v1.1
 SALT1   =  SGTE Molten Salts Database v1.2
 SEMC2   =  TC Semi-Conductors  v2.1
 SLAG4   =  Fe-containing Slag  v4.1
 SLAG3   =  Fe-containing Slag  v3.2
 SLAG2   =  Fe-containing Slag  v2.2
 SLAG1   =  Fe-containing Slag  v1.2
 TCOX10  =  Metal Oxide Solutions  v10.0
 TCOX9   =  Metal Oxide Solutions  v9.0
 TCOX8   =  Metal Oxide Solutions  v8.0
 TCOX7   =  Metal Oxide Solutions  v7.0
 TCOX6   =  Metal Oxide Solutions  v6.0
 TCOX5   =  Metal Oxide Solutions  v5.1
 TCOX4   =  Metal Oxide Solutions  v4.1
 ION3    =  Ionic Solutions  v3.0
 ION2    =  Ionic Solutions  v2.6
 ION1    =  Ionic Solutions  v1.5
 NOX2    =  NPL Oxide Solutions Database v2.1
 TCNOBL1 =  Noble Metals Alloys v1.0
```

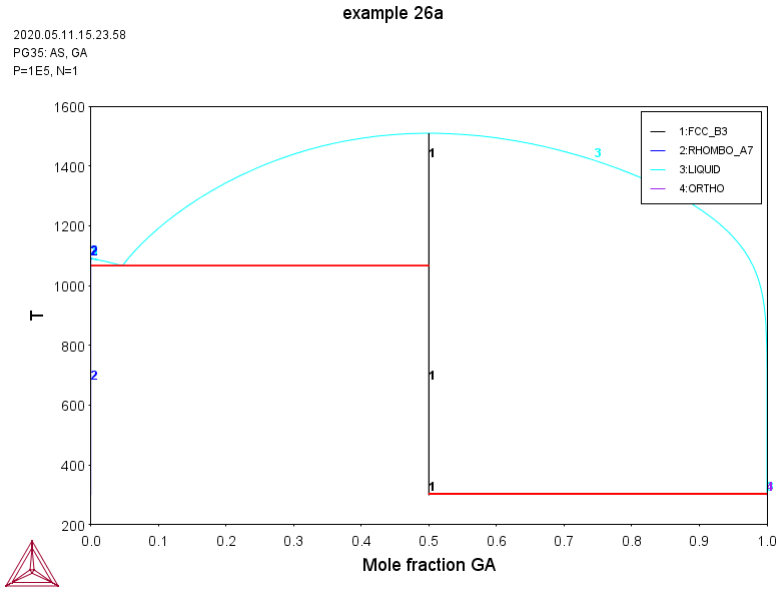
```
 TCSLD3  =  Solder Alloys  v3.3
 TCSLD2  =  Solder Alloys  v2.0
 TCSLD1  =  Solder Alloys  v1.1
 TCSI1   =  Ultrapure Silicon  v1.2
 TCMP2   =  Materials Processing  v2.5
 TCES1   =  Combustion/Sintering  v1.1
 TCSC1   =  Super Conductor  v1.0
 TCFC1   =  SOFC Database v1.0
 TCNF2   =  Nuclear Fuels  v2.1b
 NUMT2   =  Nuclear Materials  v2.1
 NUOX4   =  Nuclear Oxides  v4.2
 NUCL15  =  IRSN NUCLEA-15_4
 NUCL10  =  ThermoData NUCLEA Alloys-oxides TDB v10.2
 MEPH15  =  IRSN Mephista-15_1
 MEPH11  =  ThermoData MEPHISTA Nuclear Fuels TDB v11.2
 TCAQ3   =  Aqueous Solution  v3.0
 TCAQ2   =  Aqueous Solution  v2.7
 AQS2    =  TGG Aqueous Solution Database v2.6
 GCE2    =  TGG Geochemical/Environmental TDB v2.3
 FEDEMO  =  Iron Demo Database v3.0
 ALDEMO  =  Aluminum Demo Database v4.0
 NIDEMO  =  Nickel Demo Database v2.0
 CUDEMO  =  Copper Demo Database v1.0
 SLDEMO  =  Solder Demo Database v1.0
 OXDEMO  =  Oxide Demo Database v3.0
 SUBDEMO =  Substance Demo Database v1.0
 PTERN   =  Public Ternary Alloys TDB v1.3
 PAQ2    =  Public Aqueous Soln (SIT) TDB v2.4
 PG35    =  G35 Binary Semi-Conductors TDB v1.2
 PURE5   =  SGTE Unary (Pure Elements) TDB v5.1
 MOB2    =  Alloys Mobility  v2.7
 MOB1    =  Alloys Mobility  v1.3
 MOBFE1  =  Steels/Fe-Alloys Mobility  v1.1
 MOBFE2  =  Steels/Fe-Alloys Mobility  v2.0
 MOBFE3  =  Steels/Fe-Alloys Mobility  v3.0
 MOBFE4  =  Steels/Fe-Alloys Mobility  v4.0
 MOBFE5  =  Steels/Fe-Alloys Mobility  v5.0
 MOBNI5  =  Ni-Alloys Mobility  v5.1
 MOBNI4  =  Ni-Alloys Mobility  v4.1
 MOBNI3  =  Ni-Alloys Mobility  v3.2
 MOBNI2  =  Ni-Alloys Mobility  v2.4
 MOBNI1  =  Ni-Alloys Mobility  v1.10
 MOBAL5  =  Al-Alloys Mobility  v5.0
 MOBAL4  =  Al-Alloys Mobility  v4.0
 MOBAL3  =  Al-Alloys Mobility  v3.0
 MOBAL2  =  Al-Alloys Mobility  v2.0
 MOBAL1  =  Al-Alloys Mobility  v1.0
 MOBCU1  =  Cu-Alloys Mobility  v1.0
 MOBCU2  =  Cu-Alloys Mobility  v2.0
 MOBCU3  =  Cu-Alloys Mobility  v3.0
 MOBHEA1 =  High Entropy Alloys Mobility  v1.0
 MOBHEA2 =  High Entropy Alloys Mobility  v2.0
 MOBMG1  =  Mg-Alloys Mobility  v1.0
 MOBSI1  =  Si-Alloys Mobility  v1.0
 MOBSLD1 =  Solder-Alloys Mobility  v1.1
 MOBTI3  =  Ti-Alloys Mobility  v3.0
 MOBTI2  =  Ti-Alloys Mobility  v2.0
 MOBTI1  =  Ti-Alloys Mobility  v1.0
 MALDEMO =  Al-Alloys Mobility demo database v2.0
 MFEDEMO =  Fe-Alloys Mobility demo database v2.0
 MNIDEMO =  Ni-Alloys Mobility demo database v1.0
 MCUDEMO =  Cu-Alloys Mobility demo database v1.0
 USER    =  User defined Database

DATABASE NAME /TCFE10/: pg35
 Current database: G35 Binary Semi-Conductors TDB v1.2

 VA  DEFINED
 AL1G                    AL2G                    ALASG
 ALPG                    ALP2G                   ALSBG
   REJECTED
 AS1G                    ASGAG                   ASING
 AS2G                    AS3G                    AS4G
   REJECTED
 GA1G                    GA2G                    GAPG
 GASBG                   GASB2G  REJECTED
 IN1G                    IN2G                    INPG
 INSBG                   INSB2G  REJECTED
 P1G                     P2G                     P4G
 SB1G                    SB2G                    SB3G
 SB4G  REJECTED
TDB_PG35: d-sys as ga
   ... the command in full is DEFINE_SYSTEM
 AS                      GA  DEFINED
TDB_PG35: @@ Reject all but the stable phases in this system
TDB_PG35: rej ph /all
   ... the command in full is REJECT
 GAS:G                   LIQUID                  FCC_A1
 HCP_A3                  FCC_B3                  BCT_A5
 BCT_A6                  P_RED                   ASP
 RHOMBO_A7               ORTHO                   GA_GAMMA
   REJECTED
TDB_PG35: rest ph liq rhom ortho fcc_b3 gas:g
   ... the command in full is RESTORE
 LIQUID                  RHOMBO_A7               ORTHO
 FCC_B3                  GAS:G  RESTORED
TDB_PG35: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
 GAS:G       :AS1 AS2 AS3 AS4 AS1GA1 GA1 GA2:
  > Gaseous mixture phase: using the Ideal EOS & Mixing Model
 LIQUID      :AS GA:
  > Liquid mixture phase: Metallic species Al-As-Ga-In-P-Sb
 FCC_B3      :GA:AS:
  > FCC_B3 solution phase: for the complete Al-As-Ga-In-P-Sb system
 RHOMBO_A7   :AS:
  > RHOMBO_A7 solution phase: for the As-Sb binary join only
 ORTHO       :GA:
TDB_PG35:Hit RETURN to continue
TDB_PG35: get
   ... the command in full is GET_DATA
15:23:49,592 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
```

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

 List of references for assessed data

  'PG35 - ISC Group III-V Binary Simiconductors Database (V1.2), developed
      by Informal cientific Collaboration Group (Ansara I., Chatillon C.,
      Lukas H.L., Nishizawa T., Ohtani H., Ishida K., Hillert M., Sundman B.,
       Argent B.B., Watson A., Chart T. G., and Anderson T.), 1994, as
      published data [A Binary Database for III-V Compound Semiconductor
      Systems, Calphad, 18, 177-222] and provided by Thermo-Calc Software
      (May 2003/June 2008). '
 -OK-
TDB_PG35: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ Set conditions at the As rich side of the system. We want

POLY: @@ to calculate the metastable system without gas phase but
POLY: @@ then plot the gas constitution. Set gas to be dormant.
POLY:
POLY: s-c t=1200 p=1e5 n=1 x(ga)=.3
   ... the command in full is SET_CONDITION
POLY: c-s p gas=dor
   ... the command in full is CHANGE_STATUS
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           212 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: x
 Output from POLY-3, equilibrium =     1, label A0  , database: PG35

 Conditions:
 T=1200, P=1E5, N=1, X(GA)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1200.00 K (   926.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  7.33623E+01
 Total Gibbs energy -8.75968E+04,  Enthalpy  1.20850E+04,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 AS                      7.0000E-01  7.0000E-01 1.2211E-03 -6.6929E+04 SER
 GA                      3.0000E-01  3.0000E-01 1.2244E-06 -1.3582E+05 SER

 GAS                         Status DORMANT     Driving force  8.1507E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 AS  1.00000E+00  GA  9.09718E-11
 Constitution:
 AS4     9.80210E-01  AS3     2.00768E-03  GA1     3.55191E-10  GA2     1.87160E-17
 AS2     1.77817E-02  AS1     2.30505E-07  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:Hit RETURN to continue
POLY: @@ Note that the gas would like to be stable (driving force
POLY: @@ positive) but it is not allowed to form as it is dormant.
POLY:
POLY: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 LIQUID                  ENTERED      0.000000E+00    5.057539E-01
 FCC_B3                  ENTERED      0.000000E+00    4.942461E-01
 RHOMBO_A7               ENTERED     -4.059045E-01    0.000000E+00
 ORTHO                   ENTERED     -6.644230E+00    0.000000E+00
 GAS                     DORMANT      8.150658E-01
POLY: @@ The phase diagram is calculated with the composition and
POLY: @@ temperature on the axis as usual
POLY: 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: 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: @@ For an explanation of these symbols see below
POLY: ent fun pas1=0.4343*lnacr(as1,gas);
   ... the command in full is ENTER_SYMBOL
POLY: ent fun pas2=0.4343*lnacr(as2,gas);
   ... the command in full is ENTER_SYMBOL
POLY: ent fun pas3=0.4343*lnacr(as3,gas);
   ... the command in full is ENTER_SYMBOL
POLY: ent fun pas4=0.4343*lnacr(as4,gas);
   ... the command in full is ENTER_SYMBOL
POLY: ent fun pasga=0.4343*lnacr(as1ga1,gas);
   ... the command in full is ENTER_SYMBOL
POLY: ent fun pga1=0.4343*lnacr(ga1,gas);
   ... the command in full is ENTER_SYMBOL
POLY: ent tab pp
   ... the command in full is ENTER_SYMBOL
Variable(s): pas1 pas2 pas3 pas4 pasga pga1;
POLY:
POLY: 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)
```

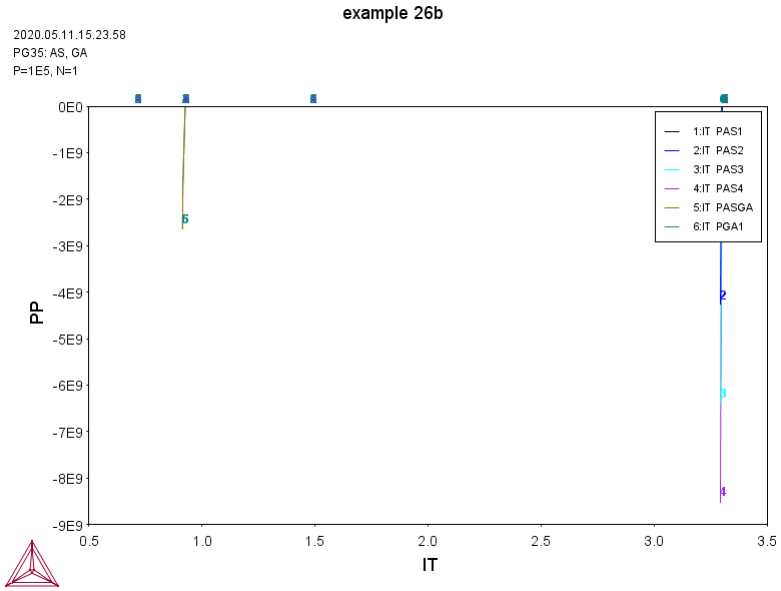
```
    PASGA=.4343*LNACR(AS1GA1,GAS)
    PGA1=.4343*LNACR(GA1,GAS)
 DEFINED TABLES
    PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
POLY:Hit RETURN to continue
POLY: ent fun dd=0.4343*dgf(gas);
   ... the command in full is ENTER_SYMBOL
POLY: ent fun qas1=log10(y(gas,as1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY: ent fun qas2=log10(y(gas,as2))+dd;
   ... the command in full is ENTER_SYMBOL
POLY: ent fun qas3=log10(y(gas,as3))+dd;
   ... the command in full is ENTER_SYMBOL
POLY: ent fun qas4=log10(y(gas,as4))+dd;
   ... the command in full is ENTER_SYMBOL
POLY: ent fun qasga=log10(y(gas,as1ga1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY: ent fun qga1=log10(y(gas,ga1))+dd;
   ... the command in full is ENTER_SYMBOL
POLY: ent tab qq
   ... the command in full is ENTER_SYMBOL
Variable(s): qas1 qas2 qas3 qas4 qasga qga1;
POLY:
POLY: ent fun it=1000/T;
   ... the command in full is ENTER_SYMBOL
POLY: save tcex26 y
   ... the command in full is SAVE_WORKSPACES
POLY: 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:Hit RETURN to continue
POLY: @@ Map follows all lines in the phase diagram
POLY: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

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

 Phase region boundary   1 at:   2.500E-01  3.100E+02
  ** FCC_B3
     RHOMBO_A7
 Calculated..                      2 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   2.500E-01  3.000E+02
  ** FCC_B3
     RHOMBO_A7
 Calculated.                      32 equilibria

 Phase region boundary   3 at:   2.500E-01  1.067E+03
  ** FCC_B3
  ** LIQUID
     RHOMBO_A7
```

```
Phase region boundary   4 at:   2.345E-02  1.067E+03
 ** LIQUID
    RHOMBO_A7
Calculated                     10 equilibria

Phase region boundary   5 at:   2.734E-01  1.067E+03
    FCC_B3
 ** LIQUID
Calculated.                    101 equilibria

Phase region boundary   6 at:   7.500E-01  3.029E+02
    FCC_B3
 ** LIQUID
 ** ORTHO

Phase region boundary   7 at:   7.500E-01  3.029E+02
    FCC_B3
 ** ORTHO
Calculated..                     2 equilibria
Terminating at axis limit.

Phase region boundary   8 at:   1.000E+00  3.029E+02
    LIQUID
 ** ORTHO
Calculated                     12 equilibria

Phase region boundary   9 at:   2.500E-01  3.100E+02
 ** FCC_B3
    RHOMBO_A7
Calculated.                     32 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   2.500E-01  3.100E+02
 ** FCC_B3
    RHOMBO_A7
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  11 at:   2.500E-01  3.100E+02
 ** FCC_B3
    RHOMBO_A7
Calculated.                     32 equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   2.500E-01  3.100E+02
 ** FCC_B3
    RHOMBO_A7
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  13 at:   2.500E-01  3.100E+02
 ** FCC_B3
    RHOMBO_A7
Calculated.                     32 equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                    100 equilibria
Terminating at known equilibrium

Phase region boundary  16 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                    100 equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.500E-01  3.100E+02
 ** FCC_B3
    LIQUID
Calculated.                    100 equilibria
Terminating at known equilibrium

Phase region boundary  20 at:   2.500E-01  8.700E+02
 ** FCC_B3
    RHOMBO_A7
Calculated..                     24 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  21 at:   2.500E-01  8.700E+02
 ** FCC_B3
    RHOMBO_A7
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   7.492E-01  8.700E+02
 ** FCC_B3
    LIQUID
Calculated.                     24 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.492E-01  8.700E+02
 ** FCC_B3
    LIQUID
```

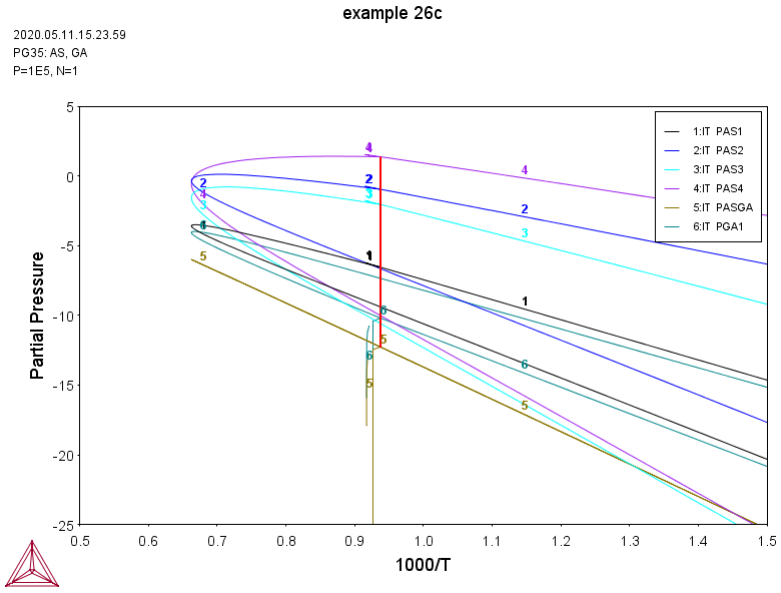
```
 Calculated.                     81 equilibria
 Terminating at known equilibrium

 Phase region boundary  24 at:   3.939E-01  1.430E+03
  ** FCC_B3
     LIQUID
 Calculated.                     18 equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   3.939E-01  1.430E+03
  ** FCC_B3
     LIQUID
 Calculated.                     87 equilibria
 Terminating at known equilibrium

 Phase region boundary  26 at:   6.143E-01  1.430E+03
  ** FCC_B3
     LIQUID
 Calculated.                     50 equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   6.143E-01  1.430E+03
  ** FCC_B3
     LIQUID
 Calculated.                     55 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   5.000E-03  1.086E+03
     LIQUID
  ** RHOMBO_A7
 Calculated                     15 equilibria

 Phase region boundary  29 at:   5.000E-03  1.086E+03
     LIQUID
  ** RHOMBO_A7
 Calculated.                      3 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   4.183E-01  1.463E+03
  ** FCC_B3
     LIQUID
 Calculated.                     21 equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   4.183E-01  1.463E+03
  ** FCC_B3
     LIQUID
 Calculated.                     67 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   5.817E-01  1.468E+03
  ** FCC_B3
     LIQUID
 Calculated.                     34 equilibria
 Terminating at known equilibrium

 Phase region boundary  33 at:   5.817E-01  1.468E+03
  ** FCC_B3
     LIQUID
 Calculated.                     54 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   7.450E-01  9.995E+02
  ** FCC_B3
     LIQUID
 Calculated.                     74 equilibria
 Terminating at known equilibrium

 Phase region boundary  35 at:   7.450E-01  9.995E+02
  ** FCC_B3
     LIQUID
 Calculated.                     29 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex26\tcex26.POLY3
 CPU time for mapping                    4 seconds
POLY: @@ Now we plot this in the post processor
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x m-f ga
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 26a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ This is the traditional phase diagram.
POST:
POST: @@ Now those who work with this system is interesting to
POST: @@ know the partial pressures of the different gas species
POST: @@ along the solubility lines. As Thermo-Calc saves the
POST: @@ complete description of all tie-lines calculated in a
POST: @@ MAP or STEP command, even for dormat phases, we can
POST: @@ now plot these.
POST:
POST: @@ The partial pressures of a species in the gas is equal
POST: @@ to the fraction of that species if the gas is stable
POST: @@ (Dalton's law). If the gas is not stable then add the
POST: @@ driving force per formula unit of the gas (the formula
POST: @@ unit depends on the species).
POST:
POST: @@ We can directly get the activity of a gas species using
POST: @@ the state variable acr(species,gas) which has as
POST: @@ reference state a pure gas of the species itself. The
POST: @@ state variable lnacr(species,gas) is the natural logarithm
POST: @@ of this quantity. To make it into log10, multiply by 0.4343
POST:
POST: s-d-a y pp
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: @@ Plot againt the inverse of temperature
POST: s-d-a x it
   ... the command in full is SET_DIAGRAM_AXIS
POST: l-sy
   ... the command in full is LIST_SYMBOLS
 DEFINED CONSTANTS
    ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    PAS1=.4343*LNACR(AS1,GAS)
    PAS2=.4343*LNACR(AS2,GAS)
    PAS3=.4343*LNACR(AS3,GAS)
    PAS4=.4343*LNACR(AS4,GAS)
    PASGA=.4343*LNACR(AS1GA1,GAS)
    PGA1=.4343*LNACR(GA1,GAS)
    DD=.4343*DGF(GAS)
    QAS1= LOG10(Y(GAS,AS1) )+DD
    QAS2= LOG10(Y(GAS,AS2) )+DD
    QAS3= LOG10(Y(GAS,AS3) )+DD
    QAS4= LOG10(Y(GAS,AS4) )+DD
    QASGA= LOG10(Y(GAS,AS1GA1) )+DD
    QGA1= LOG10(Y(GAS,GA1) )+DD
    IT=1000/T
    TEMP_C=T-273.15
 DEFINED TABLES
    PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
    QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POST: set-title example 26b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Now make the plot readable by adding axis text and labels
POST: s-s x n 0.5 1.5
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n -25 5
   ... the command in full is SET_SCALING_STATUS
POST: s-a-text x n 1000/T
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-text y n Partial Pressure
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 26c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-interactive
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex27

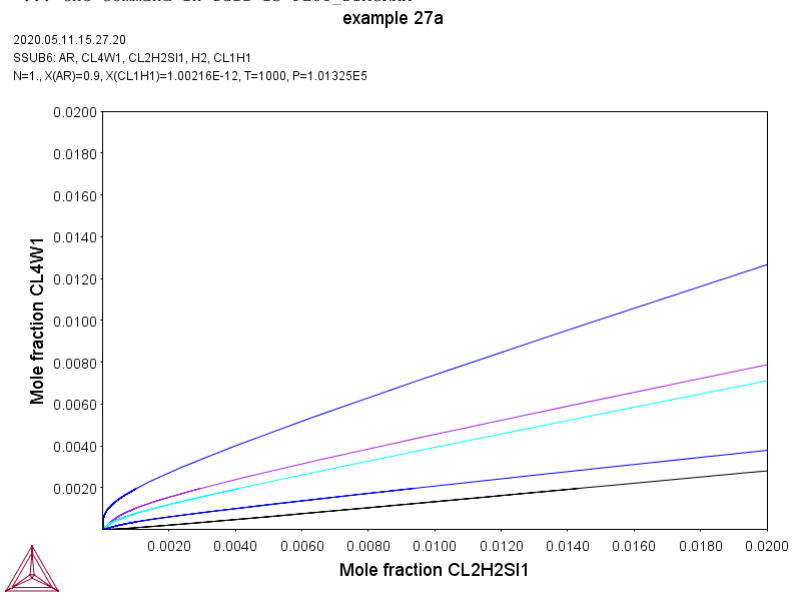
```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex27\tcex27.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating chemical vapor depositions (CVD)
SYS:
SYS: @@ Note that a SSUB database license is required
SYS: @@ to run the example.
SYS:
SYS: @@ Get data from the database
SYS: set-log ex27,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw ssub6
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v6.0

 VA  DEFINED
TDB_SSUB6:
TDB_SSUB6: d-sys h cl ar w si
   ... the command in full is DEFINE_SYSTEM
 H                       CL                      AR
 W                       SI  DEFINED
TDB_SSUB6: get
   ... the command in full is GET_DATA
15:25:18,598 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   AR1<G> HULTGREN SELECTED VAL 1973 SGTE **
      AR1<G> Ar<G>
      ARGON <GAS>
      STANDARD STATE : CODATA KEY VALUE .
   CL1<G> T.C.R.A.S. Class: 1
      CL1<G> Cl<G>
      CHLORINE <MONATOMIC GAS>
   CL10W2<G> JANAF THERMOCHEMICAL TABLES SGTE
      CL10W2<G> W2Cl10<G>
      TUNGSTEN PENTACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   CL1H1<G> T.C.R.A.S. Class: 1
      CL1H1<G> HCl<G>
      HYDROGEN CHLORIDE <GAS>
   CL1H1SI1<G> T.C.R.A.S. Class: 5
      CL1H1SI1<G>
   CL1H3SI1<G> R.W.T.H.-91 SGTE **
      CL1H3SI1<G> SiH3Cl<G>
      MOLWT(G/M): 66.5630
   CL1SI1<G> T.C.R.A.S. Class: 1
      CL1SI1<G> SiCl<G>
      SILICON MONOCHLORIDE <GAS>
   CL1W1<G> T.C.R.A.S. Class: 3
      CL1W1<G> WCl<G>
      TUNGSTEN MONOCHLORIDE <GAS>
   CL2<G> T.C.R.A.S. Class: 1
      CL2<G> Chlorine
      CHLORINE <DIATOMIC GAS>
   CL2H2SI1<G> THERMODATA 01/93
      CL2H2SI1<G> SiH2Cl2<G>
      DICHLOROSILANE
      28/01/93 DICHLOROSILANE.
   CL2SI1<G> T.C.R.A.S. Class: 5
      CL2SI1<G> SiCl2<G>
      SILICON DICHLORIDE <GAS>
   CL2W1<G> JANAF THERMOCHEMICAL TABLES SGT
      CL2W1<G> WCl2<G>
      TUNGSTEN DICHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   CL3H1SI1<G> THERMODATA 01/93
      CL3H1SI1<G> SiHCl3<G>
      28/01/93
   CL3SI1<G> T.C.R.A.S. Class: 6
      CL3SI1<G> SiCl3<G>
      SILICON TRICHLORIDE <GAS>
   CL3W1<G> T.C.R.A.S. Class: 6
      CL3W1<G>
   CL4SI1<G> T.C.R.A.S. Class: 6
      CL4SI1<G> SiCl4<G>
      SILICON TETRACHLORIDE <GAS>
   CL4W1<G> JANAF THERMOCHEMICAL TABLES SGTE
      CL4W1<G> WCl4<G>
      TUNGSTEN TETRACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   CL5W1<G> JANAF THERMOCHEMICAL TABLES SGTE
      CL5W1<G> WCl5<G>
      TUNGSTEN PENTACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
```

```
   CL6W1<G> JANAF THERMOCHEMICAL TABLES SGTE
      CL6W1<G> WCl6<G>
      TUNGSTEN HEXACHLORIDE <GAS>
      PUBLISHED BY JANAF AT 12/66
   H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
      H1<G> H<G>
      HYDROGEN <MONATOMIC GAS>
   H1SI1<G> T.C.R.A.S. Class: 2
      H1SI1<G> SiH<G>
      SILICON MONOHYDRIDE <GAS>
   H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
      H2<G> H2<G>
      HYDROGEN<G>
      STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
   H2SI1<G> T.C.R.A.S. Class: 6
      H2SI1<G>
   H3SI1<G> T.C.R.A.S. Class: 5
      H3SI1<G>
   H4SI1<G> JANAF 1978; ASSESSMENT DATED 6/76 SGTE
      H4SI1<G> SiH4<G>
      SILANE <GAS>
   H6SI2<G> THERMODATA 01/93
      H6SI2<G> Si2H6<G>
      DISILANE <GAS>
      28/01/93
   SI1<G> T.C.R.A.S. Class: 1
      SI1<G> Si<G>
      SILICON <GAS>
   SI2<G> T.C.R.A.S. Class: 5
      SI2<G> Si2<G>
      SILICON <DIATOMIC GAS>
   SI3<G> T.C.R.A.S. Class: 6
      SI3<G> Si3<G>
      SILICON <TRIATOMIC GAS>
   W1<G> T.C.R.A.S. Class: 4
      W1<G> W<G>
      TUNGSTEN <GAS>
   CL2W1 JANAF THERMOCHEMICAL TABLES SGTE **
      CL2W1 WCl2
      TUNGSTEN DICHLORIDE
      PUBLISHED BY JANAF AT 12/66
      Decomposes and sublimes to complex vapour at about 860K.
   CL3W1 T.C.R.A.S. Class: 7
      CL3W1
   CL4SI1<L> N.P.L. SGTE **
      CL4SI1 SiCl4
      SILICON TETRACHLORIDE
      ESTIM.COEF.FOR CP .MELTING PT. AT 203.15 K. LF=1850(#100)CAL/MOL FOR
      GAS
      SEE SI1CL4<G> ABOVE 331 K.
   CL4W1 JANAF THERMOCHEMICAL TABLES SGTE
      CL4W1 WCl4
      TUNGSTEN TETRACHLORIDE
      PUBLISHED BY JANAF AT 12/66
      Decomposes at 771K to WCl2(s) and WCl5(g).
   CL5W1 JANAF THERMOCHEMICAL TABLES SGTE
      CL5W1 WCl5
      TUNGSTEN PENTACHLORIDE
      PUBLISHED BY JANAF AT 12/66
   CL6W1 THERMODATA 01/93
      CL6W1 WCl6
      TUNGSTEN HEXACHLORIDE
      28/01/93 Tb = 613.6 K
   H6SI2 THERMODATA 06/86 BK
      DISILANE. Solid Standard State.
   SI2W1 VAHLAS ET AL **
      SI2W1 WSi2
      from Vahlas et al Calphad 13(3) (1989) 273
   SI3W5 VAHLAS ET AL **
      SI3W5 W5Si3
      from Vahlas et al Calphad 13(3) (1989) 273
   SI1 JANAF THERMOCHEMICAL TABLES SGTE **
      SI1 Si
      SILICON
      PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
      --U.D. 31/10/85
   W1 S.G.T.E. **
      W1 W
      Data from SGTE Unary DB
 -OK-
TDB_SSUB6:
TDB_SSUB6: @@ Calculations are made in POLY-3 module
TDB_SSUB6: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:

POLY: @@ Very many stoichiometric phases can make equilibrium calculations
POLY: @@ difficult. Setting a very high maximum number of grid points can
POLY: @@ avoid this.
POLY: adv g y 10000000
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY:
POLY: @@ In POLY-3 you define new components
POLY: def-com ar cl4w1 cl2h2si1 h2 cl1h1
   ... the command in full is DEFINE_COMPONENTS
POLY: 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:Hit RETURN to continue
POLY:
POLY: @@ Set conditions for input of gases. The best way is
POLY: @@ to set amounts equal to moles/minutes, for example.
POLY: @@ In this case we had initial partial pressures of
POLY: @@ argon 0.9 atm, WCL4 1e-5..0.1 SiH2Cl2 1e-5..0.1 unknown
POLY: @@ presure of H2. Should be no addition of HCl nor Cl but
```

```
POLY: @@ added a small addition of  Cl1H1 to get equilibrium to
POLY: @@ converge.
POLY: s-c n=1 x(ar)=.9 x(cl2h2si)=1e-3 x(cl4w)=.001 x(cl1h1)=1e-12
   ... the command in full is SET_CONDITION
POLY:
POLY: @@ At the reaction zone T=1000 and total pressure is 1 atm
POLY: s-c t=1000 p=101325
   ... the command in full is SET_CONDITION
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
    P=1.01325E5
 DEGREES OF FREEDOM 0
POLY:
POLY: @@ Save the file, then calculate and list the results
POLY: save tcex27 y
   ... the command in full is SAVE_WORKSPACES
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated       8347817 grid points in            35 s
Found the set of lowest grid points in              2 s
 Calculated POLY solution       0 s, total time    37  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB6

 Conditions:
 N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
    P=1.01325E5
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.013250E+05
 Number of moles of components  1.00000E+00,  Mass in grams  3.65774E+01
 Total Gibbs energy -1.67561E+05,  Enthalpy  1.45855E+04,  Volume  8.21892E-02

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AR                      9.0000E-01  9.8293E-01 2.0867E-09 -1.6619E+05 SER
 CL4W1                   1.0000E-03  8.9034E-03 8.9672E-57 -1.0730E+06 SER
 CL2H2SI1                1.0000E-03  2.7615E-03 1.5207E-40 -7.6231E+05 SER
 H2                      9.8000E-02  5.4008E-03 2.4479E-09 -1.6486E+05 SER
 CL1H1                   1.0022E-12  9.9901E-13 1.9600E-18 -3.3901E+05 SER

 GAS                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.0016E+00, Mass 3.6377E+01, Volume fraction 1.0000E+00  Mass fractions:
 AR        9.88357E-01  CL1H1     5.21203E-03  CL4W1     1.31332E-10
 H2        5.31980E-03  CL2H2SI1  1.11068E-03
 Constitution:
 AR        8.98562E-01  CL        3.03070E-11  H1SI1     1.54528E-17
 H2        9.65533E-02  CL1H1SI1  2.25619E-11  SI        2.70199E-19
 CL1H1     4.48535E-03  CL2W1     1.46463E-11  H6SI2     1.36833E-22
 CL4SI1    3.16220E-04  H4SI1     6.03281E-12  CL5W1     4.37795E-24
 CL3H1SI1  7.81990E-05  CL1SI1    1.41372E-12  SI2       1.26468E-26
 CL1H3SI1  4.29796E-06  CL2       6.15724E-15  CL1W1     1.35601E-30
 CL2H2SI1  3.50040E-07  H3SI1     4.22110E-16  SI3       1.15600E-30
 CL2SI1    2.90182E-07  H2SI1     3.80095E-16  W         1.00000E-30
 CL3SI1    3.29494E-09  CL4W1     1.12601E-16  CL10W2    1.00000E-30
 H         7.01220E-10  CL3W1     1.62069E-17  CL6W1     1.00000E-30

 SI3W5_S                    Status ENTERED     Driving force  0.0000E+00
 Moles-1.6000E-03, Mass 2.0070E-01, Volume fraction 0.0000E+00  Mass fractions:
 CL4W1     1.62262E+00  H2        2.00876E-02  CL1H1    -9.44672E-01
 CL2H2SI1  3.01962E-01  AR        0.00000E+00
POLY:Hit RETURN to continue
POLY: @@ Now set axis to vary along the input amounts of WCl4
POLY: @@ and SiH2Cl2. Use a logarithmic step as the magnitudes
POLY: @@ vary. Note that a limit equal to zero should not be
POLY: @@ used with log.axis
POLY:
POLY: 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: 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: @@ Add with both direction and continuation ">" to be
POLY: @@ sure to get all lines
POLY: add
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
Direction /Default/: 2>
POLY: add -2>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: 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: li-in
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  +2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
    X(CL1H1)=1.0022113E-12, T=1000, P=101325
 No 2  -2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
    X(CL1H1)=1.0021619E-12, T=1000, P=101325
POLY:Hit RETURN to continue
POLY: @@
POLY: @@ Save again with the start point before mapping
POLY: save tcex27 y
   ... the command in full is SAVE_WORKSPACES
POLY: map
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
```

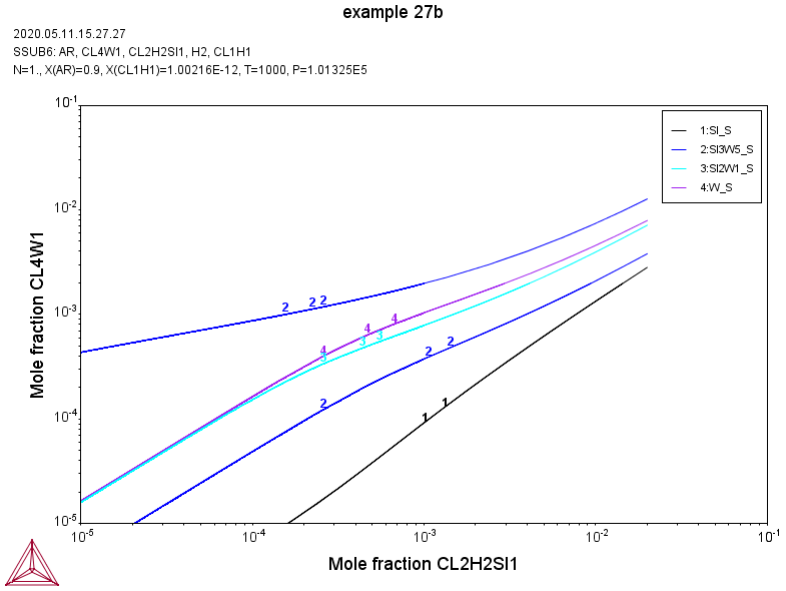
```
Generating start point   2
Generating start point   3
Generating start point   4
Generating start point   5
Generating start point   6
Generating start point   7
Generating start point   8
Generating start point   9
Generating start point  10
Working hard
Generating start point  11
Generating start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

Phase region boundary   1 at:   1.435E-02  1.970E-03
    GAS
    SI2W1_S
 ** SI_S
Calculated                      66 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                      68 equilibria

Phase region boundary   4 at:   9.344E-03  1.970E-03
    GAS
    SI2W1_S
 ** SI3W5_S
Calculated                      80 equilibria

Phase region boundary   5 at:   9.344E-03  1.970E-03
    GAS
    SI2W1_S
 ** SI3W5_S
Calculated..                       3 equilibria
Terminating at axis limit.

Phase region boundary   6 at:   2.000E-02  3.793E-03
    GAS
    SI2W1_S
 ** SI3W5_S
Calculated                      69 equilibria

Phase region boundary   7 at:   4.095E-03  1.970E-03
    GAS
 ** SI2W1_S
    SI3W5_S
Calculated                      65 equilibria

Phase region boundary   8 at:   4.095E-03  1.970E-03
    GAS
 ** SI2W1_S
    SI3W5_S
Calculated..                       4 equilibria
Terminating at axis limit.

Phase region boundary   9 at:   2.000E-02  7.114E-03
    GAS
 ** SI2W1_S
    SI3W5_S
Calculated                      70 equilibria

Phase region boundary  10 at:   2.938E-03  1.970E-03
    GAS
    SI3W5_S
 ** W_S
Calculated                      82 equilibria

Phase region boundary  11 at:   2.938E-03  1.970E-03
    GAS
    SI3W5_S
 ** W_S
Calculated..                       4 equilibria
Terminating at axis limit.

Phase region boundary  12 at:   2.000E-02  7.879E-03
    GAS
    SI3W5_S
 ** W_S
Calculated                      84 equilibria

Phase region boundary  13 at:   1.000E-03  1.970E-03
    GAS
 ** SI3W5_S
    W_S
Calculated                      92 equilibria

Phase region boundary  14 at:   1.000E-03  1.970E-03
    GAS
 ** SI3W5_S
    W_S
Calculated..                       6 equilibria
Terminating at axis limit.

Phase region boundary  15 at:   2.000E-02  1.266E-02
    GAS
 ** SI3W5_S
    W_S
Calculated                      95 equilibria

Phase region boundary  16 at:   1.000E-03  1.970E-03
    GAS
```

```
 ** SI3W5_S
    W_S
Calculated                     36 equilibria

Phase region boundary  17 at:   1.000E-03  1.970E-03
    GAS
 ** SI3W5_S
    W_S
Calculated..                      7 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   1.000E-03  1.037E-03
    GAS
    SI3W5_S
 ** W_S
Calculated                     35 equilibria

Phase region boundary  19 at:   1.000E-03  1.037E-03
    GAS
    SI3W5_S
 ** W_S
Calculated..                      6 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   1.000E-03  3.753E-04
    GAS
    SI2W1_S
 ** SI3W5_S
Calculated                     33 equilibria

Phase region boundary  21 at:   1.000E-03  3.753E-04
    GAS
    SI2W1_S
 ** SI3W5_S
Calculated..                      6 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   1.000E-03  7.855E-04
    GAS
 ** SI2W1_S
    SI3W5_S
Calculated                     33 equilibria

Phase region boundary  23 at:   1.000E-03  7.855E-04
    GAS
 ** SI2W1_S
    SI3W5_S
Calculated..                      6 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex27\tcex27.POLY3
CPU time for mapping                    27 seconds
POLY: @@
POLY: @@ Plot the diagram in the Post module
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST: set-title example 27a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

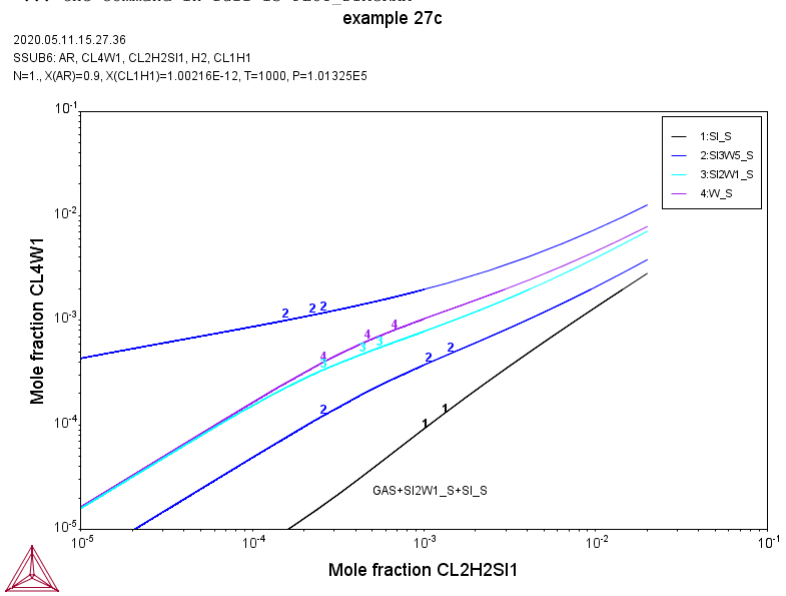



```
POST:
POST:Hit RETURN to continue
POST: @@ Better with logarithmic axis
POST: s-a-ty x log
   ... the command in full is SET_AXIS_TYPE
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-s x n 1e-5 .01
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 1e-5 .01
```

```
   ... the command in full is SET_SCALING_STATUS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: @@
POST: set-title example 27b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@Identify one of the phase regions
POST: add .0005 2e-5
   ... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
 Automatic labelling not always possible
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
 Stable phases are: GAS+SI2W1_S+SI_S
Text size: /.36/:
POST: set-title example 27c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

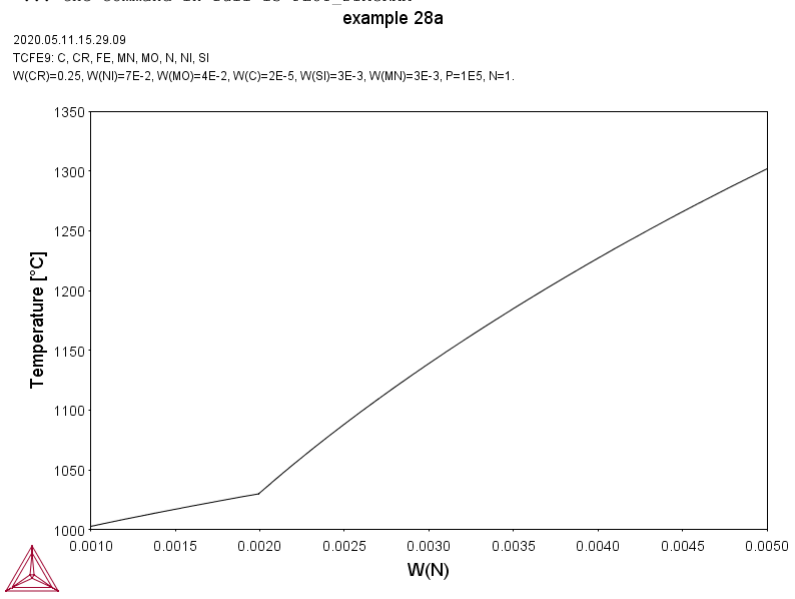
tcex28

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex28\tcex28.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Pitting Resistance Equivalence (PRE)
SYS: @@ for a duplex stainless steel.
SYS:
SYS: @@ Note that a TCFE database license is required
SYS: @@ to run the example.
SYS:
SYS: set-log ex28,,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: @@ Set the nominal composition

POLY: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: tcfe9
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: cr 25 ni 7 mo 4 c .002 n .27 si .3 mn .3
Next alloying element:
Temperature (C) /1000/: 1050
 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
 REINITIATING GES .....
   ... 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                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
 PI                      SIGMA                   HIGH_SIGMA
 MU_PHASE                P_PHASE                 R_PHASE
 CHI_A12                 LAVES_PHASE_C14         M3SI
 MN9SI2                  MN11SI19                MN6SI
 G_PHASE                 CR3SI                   FE2SI
 FESI2_H                 FESI2_L                 MSI
 M5SI3                   NBNI3                   NI3TI
 MOSI2_C11B              MO5SI3_D8M              NB5SI3_D8L
 MSI2_C40                M11SI8                  M6SI5
 AL4C3                   FE8SI2C                 SIC
 MN5SIC                  CRZN17                  CUZN_EPSILON
 BETA1                   GAMMA                   AL5FE4
 SI3N4                   MN6N4                   MN6N5
 MP_B31                  M2P_C22                 FLUORITE_C1:I
 ZRO2_TETR:I             M2O3C:I                 M2O3H:I
 CENI2                   CENI5
Reject phase(s) /NONE/: *
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
 PI                      SIGMA                   HIGH_SIGMA
 MU_PHASE                P_PHASE                 R_PHASE
 CHI_A12                 LAVES_PHASE_C14         M3SI
 MN9SI2                  MN11SI19                MN6SI
 G_PHASE                 CR3SI                   FE2SI
 FESI2_H                 FESI2_L                 MSI
 M5SI3                   NBNI3                   NI3TI
 MOSI2_C11B              MO5SI3_D8M              NB5SI3_D8L
```

```
 MSI2_C40                M11SI8                  M6SI5
 AL4C3                   FE8SI2C                 SIC
 MN5SIC                  CRZN17                  CUZN_EPSILON
 BETA1                   GAMMA                   AL5FE4
 SI3N4                   MN6N4                   MN6N5
 MP_B31                  M2P_C22                 FLUORITE_C1:I
 ZRO2_TETR:I             M2O3C:I                 M2O3H:I
 CENI2                   CENI5  REJECTED
Restore phase(s):: fcc_a1 bcc_a2 hcp_a3 m23 sigma
 FCC_A1                  BCC_A2                  HCP_A3
 M23C6                   SIGMA  RESTORED
Restore phase(s): /NONE/:

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

    The following phases are retained in this system:

 BCC_A2                   FCC_A1                   HCP_A3
 M23C6                    SIGMA

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

OK? /Y/:
15:29:00,391 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set HCP_A3#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
  'A. Fernandez Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362
      (1988); C-CO-NI AND C-CO-FE-NI'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'C. Qiu, ISIJ International, 32 (1992) 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  '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'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'J-O. Andersson, CALPHAD, 12 (1988) 1-8; TRITA 0317 (1986); C-MO'
  'J.-H. Shim, C.-S. Oh, D.N. Lee, Metall. Mater. Trans. B. 27 (1996) 955
      -966; Ti-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'
  'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
      (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
  'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
  'K. Frisk, KTH Report D 60 (1984); CR-MO'
  'B. Sundman, Private communication; FCC parameter same as BCC; Cr-Mo'
  'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
  'K. Frisk, CALPHAD, 15 (1991) 79-106; TRITA-MAC 393 (1989); CR-N, FE-N, MO
      -N, CR-MO-N'
  'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'A. Fernandez Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised
      1986); TRITA-MAC 200 (1982); FE-MO'
  'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
  'C. Qiu and A. Fernandez Guillermet, Z. Metallkd., 84 (1993) 11-12; Mn-N'
  'S. Liu, Unpublished work (2010); Mn-Ni'
  'C.P. Guo,Intermetallics,13(5),525-534,(2005); Mn-Ni'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'K. Frisk, CALPHAD, 14 (1990) 311-320; MO-NI'
  'Y. Liu, G. Shao, P. Tsakiropoulos, Intermatallics 8 (2000) 953-962; Mo-Si,
       Al-Mo-Si'
  'K. Frisk, Z. Metallkd., 82 (1991) 59-66; TRITA-MAC 414 (1989); Fe-Ni-N'
  'K. Frisk, Int. J. Thermophys., 12 (1990) 417-431; TRITA-MAC 419 (1990); N
      -NI'
  'P. Gustafson, Inst. Met. Res. (Sweden) (1990); Estimations of C-CR-FE-V,
      C-CR-FE-MO-V-W, FE-N-W, FE-MN-N, FE-N-SI, CR-N-V, C-CR-N, FE-MO-N, CR
      -N-W, CR-TI-N'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-V-W-C'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218;
      TRITA-MAC 285 (1986); C-FE-NI'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
```

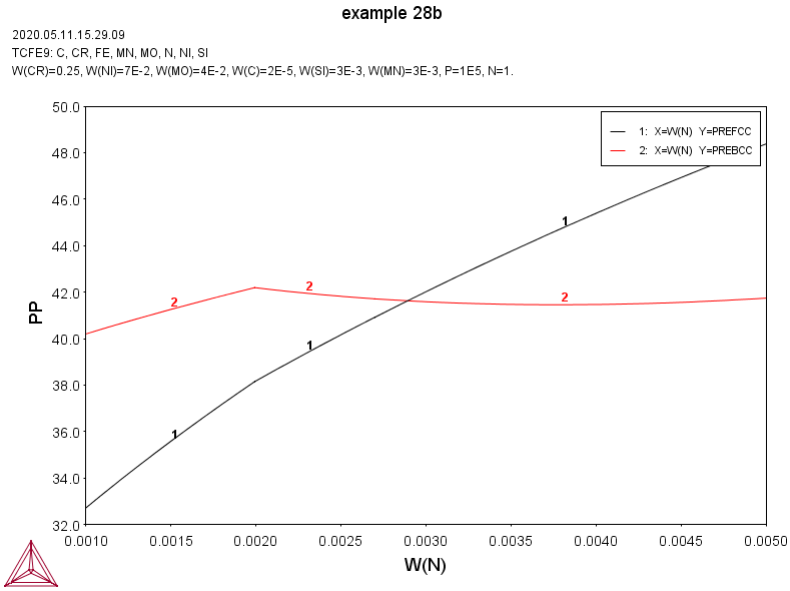
```
  'B.-J. Lee, Private communication, (2000); Estimated parameter'
  'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Fe-Cr-Ni'
  'B. Sundman, Private communication, 2(1999); Estimated parameter'
  'B. Sundman, Private communication, (2000); Estimated Cr-Ni-Mo'
  'K. Frisk, TRITA-MAC 422 (1990); CR-FE-N-NI'
  'C. Qiu, Metall. Trans. A, 24A (1993) 629-645; Fe-Mn-N'
  'L. Zhang, Y. Du, H. Xu, S. Liu, Y. Liu, F. Zheng, et al., Int. J. Mater.
      Res. 100 (2009) 160-175; Fe-Mn-Ni'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
  'K. Frisk, TRITA-MAC 433 (1990); FE-CR-MO-NI-N'
  'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
  'A. Kusoffsky et al., Work within CCT-Applied Stainless steels, 2004; Fe
      -Cr-Si, Fe-Ni-Si, Fe-Cr-Cu, Fe-Cu-Mo, Cr-Mo-N-Ni, Fe-Cr-N-Ni, Fe-Al-Cr
      -Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
      M23C6'
  'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; Fe-Cr-N, Fe
      -C-Cr-N, Fe-Cr-Mo-N, Fe-Cr-Mn-N'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated          7296 grid points in             2 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       2 s, total time     4  s
POLY:
POLY: save tcex28 y
   ... the command in full is SAVE_WORKSPACES
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -7.36324E+04,  Enthalpy  3.91744E+04,  Volume  7.43493E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 3.1563E-05 -1.1401E+05 SER
 CR                      2.6597E-01  2.5000E-01 2.5102E-03 -6.5869E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.6003E-03 -7.0822E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.8924E-06 -1.4030E+05 SER
 MO                      2.3064E-02  4.0000E-02 6.3808E-04 -8.0937E+04 SER
 N                       1.0663E-02  2.7000E-03 4.5184E-07 -1.6073E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.2158E-04 -9.9177E+04 SER
 SI                      5.9088E-03  3.0000E-03 3.2978E-09 -2.1486E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 5.5953E-01, Mass 3.0746E+01, Volume fraction 5.5498E-01  Mass fractions:
 FE  6.37043E-01  NI  8.56120E-02  N   4.58698E-03  SI  2.64555E-03
 CR  2.34717E-01  MO  3.20656E-02  MN  3.30095E-03  C   2.92454E-05

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.4047E-01, Mass 2.4572E+01, Volume fraction 4.4502E-01  Mass fractions:
 FE  6.24069E-01  NI  5.04648E-02  SI  3.44352E-03  N   3.38836E-04
 CR  2.69123E-01  MO  4.99282E-02  MN  2.62343E-03  C   8.43132E-06
POLY:
POLY:Hit RETURN to continue
POLY: @@ Calculate the temperature for an equal amount
POLY: c-s p bcc_a2=fix .5
   ... the command in full is CHANGE_STATUS
POLY: s-c t=none
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated          7296 grid points in             0 s
    11 ITS,  CPU TIME USED   1 SECONDS
POLY: sh t
   ... the command in full is SHOW_VALUE
 T=1382.343
POLY: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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   1382.34 K (  1109.19 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -7.87284E+04,  Enthalpy  4.14321E+04,  Volume  7.46368E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 2.9825E-05 -1.1976E+05 SER
 CR                      2.6597E-01  2.5000E-01 2.0891E-03 -7.0927E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.3619E-03 -7.5844E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.5787E-06 -1.4790E+05 SER
 MO                      2.3064E-02  4.0000E-02 4.8018E-04 -8.7826E+04 SER
 N                       1.0663E-02  2.7000E-03 6.6752E-07 -1.6343E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.0989E-04 -1.0477E+05 SER
 SI                      5.9088E-03  3.0000E-03 4.8855E-09 -2.1995E+05 SER

 BCC_A2                      Status FIXED       Driving force  0.0000E+00
 Moles 5.0096E-01, Mass 2.7932E+01, Volume fraction 5.0554E-01  Mass fractions:
 FE  6.26658E-01  NI  5.39523E-02  SI  3.40350E-03  N   4.72072E-04
 CR  2.64424E-01  MO  4.83843E-02  MN  2.69685E-03  C   9.16390E-06

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 4.9904E-01, Mass 2.7386E+01, Volume fraction 4.9446E-01  Mass fractions:
 FE  6.35995E-01  NI  8.63682E-02  N   4.97242E-03  SI  2.58844E-03
 CR  2.35288E-01  MO  3.14482E-02  MN  3.30921E-03  C   3.10525E-05
POLY: @@ Enter the PRE functions
POLY: ent fun prefcc
   ... the command in full is ENTER_SYMBOL
```

```
Function: 100*w(fcc_a1,cr)+300*w(fcc_a1,mo)+1600*w(fcc_a1,n);
POLY: ent fun prebcc
   ... the command in full is ENTER_SYMBOL
Function: 100*w(bcc_a2,cr)+300*w(bcc_a2,mo)+1600*w(bcc_a2,n);
POLY: 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: eval
   ... the command in full is EVALUATE_FUNCTIONS
Name(s): *
 PREFCC=40.919137
 PREBCC=41.713014
POLY:Hit RETURN to continue
POLY: @@ Then vary the nitrogen content
POLY: 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: 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: save tcex28 y
   ... the command in full is SAVE_WORKSPACES
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
 No initial equilibrium, using default
 Step will start from axis value   0.270000E-02
...OK

 Phase Region from   0.270000E-02 for:
     BCC_A2
     FCC_A1#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 check of adding phase at  1.99365E-03
 Calculated    10 equilibria

 Phase Region from   0.199365E-02 for:
     BCC_A2
     FCC_A1#1
     SIGMA
 Global test at  1.20000E-03 .... OK
 Terminating at   0.100000E-02
 Calculated    13 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex28\tcex28.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: @@ First plot how the temperature varies
POST: s-d-a x w(n)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 28a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

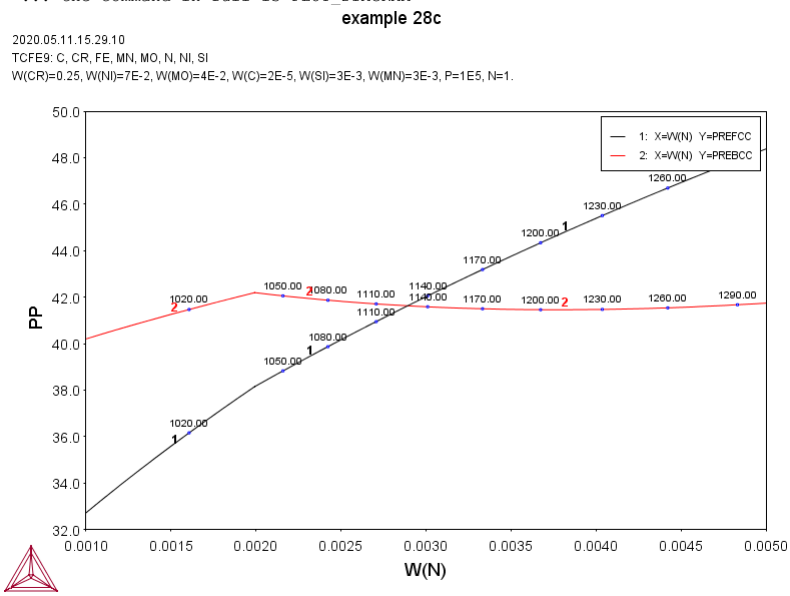



```
POST:
POST:Hit RETURN to continue
POST: @@ Then plot the PRE
POST: ent tab pp
   ... the command in full is ENTER_SYMBOL
Variable(s): prefcc prebcc
&
POST:
```

```
POST: s-d-a y pp
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 28b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Add the temperature as tic marks to the plot
POST: s-d-a z t-c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 800 1300
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 28c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: back
POLY: @@ Check how close we are to form Cr2N
POLY: read tcex28
   ... the command in full is READ_WORKSPACES
POLY:
POLY: @@ Restore BCC as entered
POLY: c-s p bcc_a2=ent 1
   ... the command in full is CHANGE_STATUS
POLY: s-c t=1323
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
```

```
Calculated          7296 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: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -7.36196E+04,  Enthalpy  3.91688E+04,  Volume  7.43486E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 3.1568E-05 -1.1400E+05 SER
 CR                      2.6597E-01  2.5000E-01 2.5114E-03 -6.5857E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.6010E-03 -7.0809E+04 SER
 MN                      3.0208E-03  3.0000E-03 2.8933E-06 -1.4029E+05 SER
 MO                      2.3064E-02  4.0000E-02 6.3855E-04 -8.0920E+04 SER
 N                       1.0663E-02  2.7000E-03 4.5138E-07 -1.6072E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.2161E-04 -9.9162E+04 SER
 SI                      5.9088E-03  3.0000E-03 3.2944E-09 -2.1484E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 5.5967E-01, Mass 3.0754E+01, Volume fraction 5.5512E-01  Mass fractions:
 FE  6.37045E-01  NI  8.56102E-02  N   4.58615E-03  SI  2.64568E-03
 CR  2.34716E-01  MO  3.20671E-02  MN  3.30093E-03  C   2.92414E-05

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.4033E-01, Mass 2.4564E+01, Volume fraction 4.4488E-01  Mass fractions:
 FE  6.24063E-01  NI  5.04560E-02  SI  3.44361E-03  N   3.38548E-04
 CR  2.69136E-01  MO  4.99319E-02  MN  2.62324E-03  C   8.42973E-06
POLY:Hit RETURN to continue
POLY: @@ Find out at which temperature sigma forms
POLY: 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          7296 grid points in             0 s
To form SIGMA the condition is set to T=1307.6676684
POLY:Hit RETURN to continue
POLY: @@ Find the temperature for Cr2N, set the start
POLY: @@ constitution. but first make sure hcp#2 is nitride
POLY: s-s-c hcp_a3#2 *
   ... the command in full is SET_START_CONSTITUTION
POLY: c-t
   ... the command in full is COMPUTE_TRANSITION
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
Phase to form: hcp_a3#2
 You must release one of these conditions
 T=1307.67, 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          7296 grid points in             0 s
To form HCP_A3 the condition is set to T=1251.46776139
POLY: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 Conditions:
 T=1251.47, 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   1251.47 K (   978.32 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.53180E+01
 Total Gibbs energy -6.76080E+04,  Enthalpy  3.59264E+04,  Volume  7.36085E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       9.2112E-05  2.0000E-05 3.4967E-05 -1.0677E+05 SER
 CR                      2.6597E-01  2.5000E-01 3.1479E-03 -5.9945E+04 SER
 FE                      6.2530E-01  6.3128E-01 1.9889E-03 -6.4723E+04 SER
 MN                      3.0208E-03  3.0000E-03 3.3132E-06 -1.3129E+05 SER
 MO                      2.3064E-02  4.0000E-02 6.9044E-04 -7.5732E+04 SER
 N                       1.0663E-02  2.7000E-03 2.6151E-07 -1.5771E+05 SER
 NI                      6.5978E-02  7.0000E-02 1.3114E-04 -9.3016E+04 SER
 SI                      5.9088E-03  3.0000E-03 2.3720E-09 -2.0664E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 7.4578E-01, Mass 4.0935E+01, Volume fraction 7.4364E-01  Mass fractions:
 FE  6.54429E-01  NI  8.11347E-02  N   3.61990E-03  MN  3.28410E-03
 CR  2.30006E-01  MO  2.40260E-02  SI  3.47485E-03  C   2.60512E-05

 SIGMA                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.5963E-01, Mass 9.1407E+00, Volume fraction 1.6043E-01  Mass fractions:
 FE  5.26062E-01  MO  1.12898E-01  MN  1.98730E-03  C   0.00000E+00
 CR  3.24159E-01  NI  3.48032E-02  SI  9.02933E-05  N   0.00000E+00

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.4597E-02, Mass 5.2426E+00, Volume fraction 9.5930E-02  Mass fractions:
 FE  6.33984E-01  NI  4.44270E-02  SI  4.36551E-03  N   2.24956E-04
 CR  2.76818E-01  MO  3.76250E-02  MN  2.54743E-03  C   7.62286E-06

 HCP_A3#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mass fractions:
 CR  8.24243E-01  MO  3.87305E-02  NI  1.28843E-03  C   2.96348E-04
 N   1.08079E-01  FE  2.66231E-02  MN  7.39264E-04  SI  2.19788E-08
POLY: @@ Rapid cooling is needed to avoid these phases.
POLY: set-inter
   ... the command in full is SET_INTERACTIVE
POLY:
```

tcex29

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex29\tcex29.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating the speciation of a gas
SYS:
SYS: @@ Note that a SSUB database license is required
SYS: @@ to run the example.
SYS:
SYS: set-log ex29,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw ssub6
   ... the command in full is SWITCH_DATABASE
 Current database: SGTE Substances Database v6.0

 VA  DEFINED
TDB_SSUB6:
TDB_SSUB6: d-sys c o h s
   ... the command in full is DEFINE_SYSTEM
 C                       O                       H
 S  DEFINED
TDB_SSUB6: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
 GAS:G       :C C1H1 C1H1O1 C1H1O2 C1H2 C1H2O1 C1H2O2_CIS C1H2O2_DIOXIRANE
  C1H2O2_TRANS C1H3 C1H3O1_CH2OH C1H3O1_CH3O C1H4 C1H4O1 C1H4S1 C1O1 C1O1S1
  C1O2 C1S1 C1S2 C2 C2H1 C2H2 C2H2O1 C2H3 C2H4 C2H4O1_ACETALDEHYDE
  C2H4O1_OXIRANE C2H4O2_ACETICACID C2H4O2_DIOXETANE C2H4O3_123TRIOXOLANE
  C2H4O3_124TRIOXOLANE C2H5 C2H6 C2H6O1_1 C2H6O1_2 C2H6O2 C2O1 C3 C3H1
  C3H4_1 C3H4_2 C3H6_1 C3H6_2 C3H6O1_1 C3H6O1_2 C3H8 C3O2 C4 C4H1 C4H10_1
  C4H10_2 C4H2_1 C4H2_2 C4H4_1 C4H4_2 C4H6_1 C4H6_2 C4H6_3 C4H6_4 C4H6_5
  C4H8_1 C4H8_2 C4H8_3 C4H8_4 C4H8_5 C4H8_6 C5 C60 C6H6 C6H6O1 H H1O1
  H1O1S1_HSO H1O1S1_SOH H1O2 H1S1 H2 H2O1 H2O1S1_H2SO H2O1S1_HSOH H2O2
  H2O4S1 H2S1 H2S2 O O1S1 O1S2 O2 O2S1 O3 O3S1 S S2 S3 S4 S5 S6 S7 S8:
 C_S         :C:
 C_L         :C:
 DIAMOND     :C:
 C1H2O2_L    :C1H2O2:
 C1H2S3_L    :C1H2S3:
 C1H4_L      :C1H4:
 C1H4O1_L    :C1H4O1:
 C1H4S1_L    :C1H4S1:
 C1S2_L      :C1S2:
 C2H4O2_L    :C2H4O2:
 C2H6_L      :C2H6:
 C2H6O1_L    :C2H6O1:
 C2H6O2_L    :C2H6O2:
 C3H6_L      :C3H6:
 C3H8_L      :C3H8:
 C4H8_L      :C4H8:
 C60_S       :C60:
 C6H6_L      :C6H6:
 H10O8S1_L   :H10O8S1:
 H15O10_5S1_L :H15O10.5S1:
 H2O1_L      :H2O1:
 H2O2_L      :H2O2:
 H2O4S1_L    :H2O4S1:
 H2S1_L      :H2S1:
 H2S2_L      :H2S2:
 H4O5S1_L    :H4O5S1:
 H6O6S1_L    :H6O6S1:
 H8O7S1_L    :H8O7S1:
 O3S1_L      :O3S1:
 S_S         :S:
 S_S2        :S:
 S_L         :S:
TDB_SSUB6:Hit RETURN to continue
TDB_SSUB6: get
   ... the command in full is GET_DATA
15:30:28,732 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
      C1<G> C<G>
   C1H1<G> T.C.R.A.S. Class: 2
      C1H1<G> CH<G>
   C1H1O1<G> T.C.R.A.S. Class: 4
      C1H1O1<G> HCO<G>
      FORMYL <GAS>
   C1H1O2<G> T.C.R.A.S. Class: 6
      C1H1O2<G>
   C1H2<G> T.C.R.A.S. Class: 5
      METHYLENE
      METHYLENE <GAS>
   C1H2O1<G> T.C.R.A.S. Class: 5
```

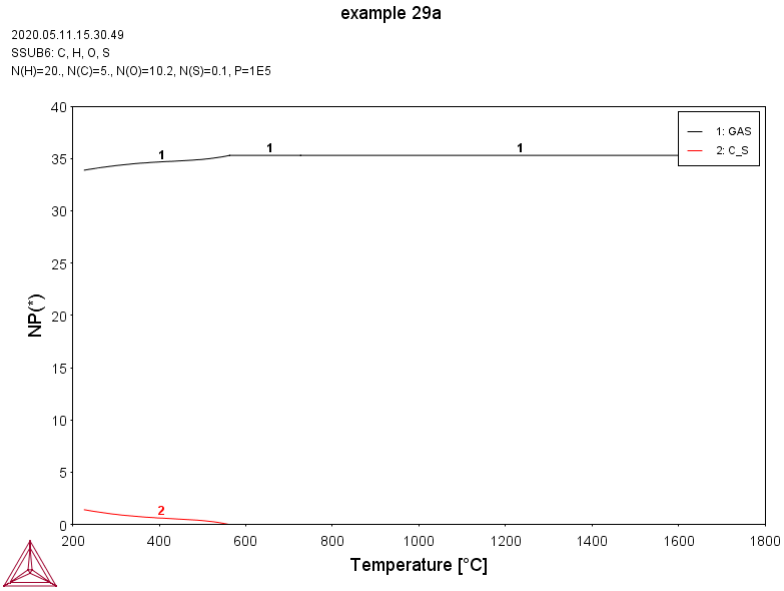
```
   C1H2O1<G> CH2O<G>
   FORMALDEHYDE <GAS>
C1H2O2_CIS<G> T.C.R.A.S. Class: 5
   C1H2O2_CIS<G>
C1H2O2_DIOXIRANE<G> T.C.R.A.S. Class: 6
   C1H2O2_DIOXIRANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C1H2O2_TRANS<G> T.C.R.A.S. Class: 5
   C1H2O2_TRANS<G>
C1H3<G> T.C.R.A.S. Class: 5
   METHYL Gaseous Standard State.
   METHYL <GAS>
C1H3O1_CH2OH<G> T.C.R.A.S. Class: 6
   C1H3O1_CH2OH<G>
C1H3O1_CH3O<G> T.C.R.A.S. Class: 5
   C1H3O1_CH3O<G>
C1H4<G> T.C.R.A.S. Class: 5
   METHANE. Gaseous Standard State.
   METHANE <GAS>
C1H4O1<G> T.C.R.A.S. Class: 5
   C1H4O1<G> CH3OH<G>
   METHANOL <GAS>
C1H4S1<G> THERMODATA 04/98 TC
   METHANETHIOL. Gaseous Standard State.
C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
   C1O1<G> CO<G>
   CARBON MONOXIDE <GAS>
   STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
C1O1S1<G> T.C.R.A.S. Class: 2
   C1O1S1<G> COS<G>
   CARBON OXIDE SULFIDE <GAS>
C1O2<G> T.C.R.A.S. Class: 2
   C1O2<G> CO2<G>
   CARBON DIOXIDE <GAS>
C1S1<G> T.C.R.A.S. Class: 1
   C1S1<G> CS<G>
   CARBON MONOSULFIDE <GAS>
C1S2<G> T.C.R.A.S. Class: 3
   C1S2<G> CS2<G>
   CARBON DISULFIDE <GAS>
C2<G> T.C.R.A.S. Class: 2
   CARBON Diatomic Gas.
   CARBON <DIATOMIC GAS>
C2H1<G> T.C.R.A.S. Class: 6
   C2H1<G> C2H<G>
   CCH RADICAL <GAS>
C2H2<G> T.C.R.A.S. Class: 2
   ACETYLENE (ETYNE). Gaseous Standard State.
   ACETYLENE <GAS>
C2H2O1<G> T.C.R.A.S. Class: 6
   C2H2O1<G>
   OXIRENE
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C2H3<G> T.C.R.A.S. Class: 6
   DICARBON TRIHYDRIDE Gaseous Standard State.
C2H4<G> T.C.R.A.S. Class: 6
   ETHYLENE. Gaseous Standard State.
   ETHYLENE <GAS>
C2H4O1_ACETALDEHYDE<G> T.C.R.A.S. Class: 5
   C2H4O1_ACETALDEHYDE<G>
C2H4O1_OXIRANE<G> T.C.R.A.S. Class: 6
   C2H4O1_OXIRANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C2H4O2_ACETICACID<G> T.C.R.A.S. Class: 5
   C2H4O2_ACETICACID<G>
C2H4O2_DIOXETANE<G> T.C.R.A.S. Class: 6
   C2H4O2_DIOXETANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
   typing error corrected 12/06
C2H4O3_123TRIOXOLANE<G> T.C.R.A.S. Class: 7
   C2H4O3_123TRIOXOLANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C2H4O3_124TRIOXOLANE<G> T.C.R.A.S. Class: 7
   C2H4O3_124TRIOXOLANE<G>
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
   typing error corrected 12/06
C2H5<G> T.C.R.A.S. Class: 6
   ETHYL radical. Gaseous Standard State.
C2H6<G> T.C.R.A.S. Class: 6
   ETHANE. Gaseous Standard State.
C2H6O1_1<G> THERMODATA 04/98 TC
   ETHANOL. Gaseous Standard State.
C2H6O1_2<G> THERMODATA 04/98 TC
   DIMETHYL ETHER. Gaseous Standard State.
C2H6O2<G> THERMODATA
   C2H6O2<G>
   E-GLYCOL <GAS>.Data revised by THDA.
C2O1<G> T.C.R.A.S. Class: 5
   C2O1<G>
C3<G> T.C.R.A.S. Class: 6
   CARBON triatomic gas.
   CARBON <TRIATOMIC GAS>
C3H1<G> T.C.R.A.S. Class: 6
   C3H1<G>
   2-PROPYNYLIDYNE
   S298 corrected and cp refitted
   due to corrected data in IVTAN2000 7/2002
C3H4_1<G> STULL WESTRUM SINKE 1969 SGTE
   C3H4_1<G>
   ALLENE = 1,2-PROPADIENE
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H4_2<G> STULL WESTRUM SINKE 1969 SGTE
   C3H4_2<G>
   PROPYNE (METHYLACETYLENE)
   EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H6O1_1<G> THERMODATA 04/98 TC
   2-PROPENOL (ALLYL ALCOHOL). Gaseous Standard State.
C3H6O1_2<G> THERMODATA 04/98 TC
   DL-METHYLOXIRANE. Gaseous Standard State.
C3H6_1<G> T.C.R.A.S. Class: 6 4.09.85
```

C3H6(G)Cyclopropane
C3H6_2<G> STULL WESTRUM SINKE 1969 SGTE
PROPENE
PROPENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C3H8<G> THERMODATA SGTE
PROPANE. Gaseous Standard State.
PROPANE <GAS>
PROPANE
C3O2<G> T.C.R.A.S. Class: 6
C3O2<G>
C4<G> T.C.R.A.S. Class: 7
C4<G>
C4H1<G> T.C.R.A.S Class: 6
1,3-BUTADIYNYL Gaseous Standard State.
1,3-BUTADIYNYL. Data provided by T.C.R.A.S. in 2000
C4H10_1<G> T.C.R.A.S Class: 4
BUTANE Gaseous Standard State.
BUTANE. Data provided by T.C.R.A.S. in 2000
C4H10_2<G> T.C.R.A.S Class: 4
METHYLPROPANE N-BUTANE Gaseous Standard State.
METHYLPROPANE N-BUTANE. Data provided by T.C.R.A.S. in 2000
C4H2_1<G> THERMODATA 1978 ST
1,3-BUTADIYNE. Gaseous Standard State.
C4H2_2<G> THERMODATA 06/93 ST
BUTADIYNE(BIACETYLENE). Gaseous Standard State.
C4H4_1<G> T.C.R.A.S Class: 6
1,3-CYCLOBUTADIENE Gaseous Standard State.
1,3-CYCLOBUTADIENE. Data provided by T.C.R.A.S. in 2000
C4H4_2<G> STULL WESTRUM SINKE 1969 SGTE
1-BUTEN-3-YNE VINYLACETYLENE. Gaseous Standard State.
1-BUTEN-3-YNE VINYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_1<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_1<G>
1,2-BUTADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_2<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_2<G>
1,3-BUTADIENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_3<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_3<G>
1-BUTYNE ETHYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_4<G> STULL WESTRUM SINKE 1969 SGTE
C4H6_4<G>
2-BUTYNE DIMETHYLACETYLENE
EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.
C4H6_5<G> T.C.R.A.S Class: 6
C4H6_5<G>
CYCLOBUTENE. Data provided by T.C.R.A.S. in 2000
C4H8_1<G> THERMODATA 04/98 TC
1-BUTENE. Gaseous Standard State.
C4H8_2<G> THERMODATA 04/98 TC
(E)-2-BUTENE. Gaseous Standard State.
C4H8_3<G> THERMODATA 04/98 TC
(Z)-2-BUTENE. Gaseous Standard State.
C4H8_4<G> THERMODATA 04/98 TC
CYCLOBUTANE. Gaseous Standard State.
C4H8_5<G> THERMODATA 04/98 TC
2-METHYLPROPENE. Gaseous Standard State.
C4H8_6<G> THERMODATA 04/98 TC
METHYLCYCLOPROPANE. Gaseous Standard State.
C5<G> T.C.R.A.S. Class: 7
C5<G>
C60<G> MHR-95
C60<G>
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the rotational
data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that
a frequency with degeneracy 5 is missing from list in [94Kor/Sid];
taken to be 419 cm-1, which gives very good, though not exact,
agreement with values quoted in [94Kor/Sid]. Note discrepancy
between calculated DrS(298) = -8943.5 J mol K-1 for the reaction
60C<g>=C60<g>and that given by [94Kor/Sid] in their Table 5,
-8950 J mol K-1. Enthalpy of formation: DfH = 2588 kJ/mol from
DsubH(298.15K) = 166 +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure
values reproduced very well.
[91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).
C6H6<G> T.C.R.A.S Class: 5
BENZENE. Gaseous Standard State.
BENZENE. Data provided by T.C.R.A.S. in 2000
C6H6O1<G> THERMODATA 01/93
C6H6O1<G>
PHENOL
28/01/93
H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE **
H1<G> H<G>
HYDROGEN <MONATOMIC GAS>
H1O1<G> T.C.R.A.S. Class: 1
H1O1<G> OH<G>
H1O1S1_HSO<G> T.C.R.A.S. Class: 4
H1O1S1_HSO<G>
H1O1S1_SOH<G> T.C.R.A.S. Class: 5
H1O1S1_SOH<G>
H1O2<G> T.C.R.A.S. Class: 4
H1O2<G>
H1S1<G> T.C.R.A.S. Class: 2
H1S1<G>
H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
H2<G> H2<G>
HYDROGEN<G>
STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
H2O1<G> T.C.R.A.S. Class: 1
H2O1<G> H2O<G>
WATER <GAS>
H2O1S1_H2SO<G> T.C.R.A.S. Class: 4
H2O1S1_H2SO<G>
H2O1S1_HSOH<G> T.C.R.A.S. Class: 4
H2O1S1_HSOH<G>
H2O2<G> JANAF SECOND EDIT SGTE
H2O2<G> H2O2<G>
HYDROGEN PEROXIDE <GAS>
H2O4S1<G> JANAF 1982; ASSESSMENT DATED 9/77 SGTE
H2O4S1<G> H2SO4<G>

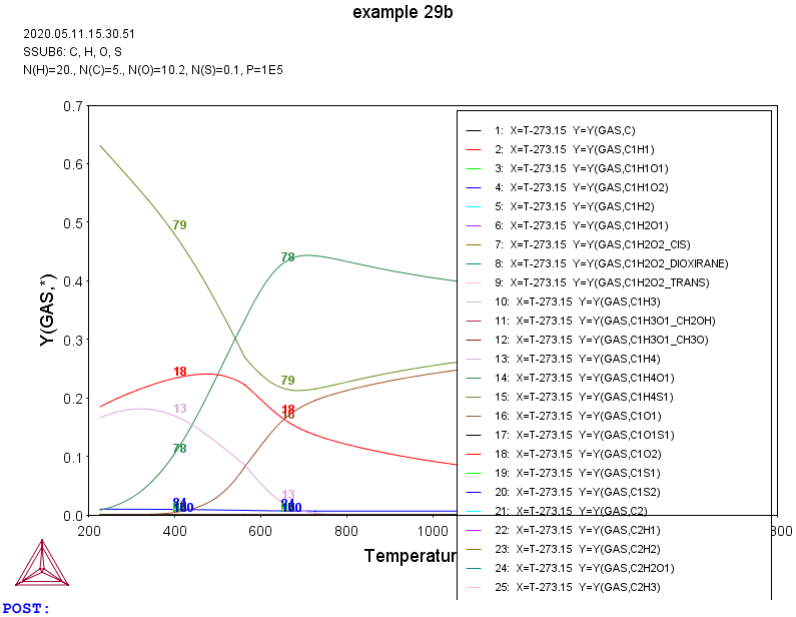
SULFURIC ACID <GAS>
H2S1<G> T.C.R.A.S. Class: 2
H2S1<G> H2S<G>
HYDROGEN SULFIDE <GAS>
H2S2<G> K.C. MILLS SGTE **
H2S2<G> H2S2<G>
DIHYDROGEN DISULFIDE <GAS>
O1<G> TCRAS 02/06/80
O1 Gaseous Standard State.
O1S1<G> T.C.R.A.S. Class: 3
O1S1<G> SO<G>
SULFUR MONOXIDE <GAS>
O1S2<G> JANAF THERMOCHEMICAL TABLES SGTE **
O1S2<G> S2O<G>
DISULFUR MONOXIDE <GAS>
PUBLISHED BY JANAF AT 9/65
O2<G> TCRAS 21/06/90
OXYGEN Gaseous Standard State.
O2S1<G> JANAF THERMOCHEMICAL TABLES SGTE **
O2S1<G> SO2<G>
SULFUR DIOXIDE <GAS>
PUBLISHED BY JANAF AT 6/61
O3<G> TCRAS 02/06/80
OZONE Gaseous Standard State.
O3S1<G> JANAF THERMOCHEMICAL TABLES SGTE **
O3S1<G> SO3<G>
SULFUR TRIOXIDE <GAS>
PUBLISHED BY JANAF AT 9/65
S1<G> T.C.R.A.S. Class: 1
S1<G> S<G>
SULFUR <GAS>
S2<G> T.C.R.A.S. Class: 4
S2<G> S2<G>
SULFUR <DIATOMIC GAS>
S3<G> T.C.R.A.S. Class: 5
S3<G> S3<G>
SULFUR <3-ATOMIC GAS>
S4<G> T.C.R.A.S. Class: 6
S4<G> S4<G>
SULFUR <4-ATOMIC GAS>
S5<G> T.C.R.A.S. Class: 6
S5<G> S5<G>
SULFUR <5-ATOMIC GAS>
S6<G> T.C.R.A.S. Class: 6
S6<G> S6<G>
SULFUR <6-ATOMIC GAS>
S7<G> T.C.R.A.S. Class: 7
S7<G> S7<G>
SULFUR <7-ATOMIC GAS>
S8<G> T.C.R.A.S. Class: 7
S8<G> S8<G>
SULFUR <OCTATOMIC GAS>
C1H2O2<L> THERMODATA 01/93
C1H2O2 HCOOH
FORMIC ACID MONOMERIC
28/01/93
C1H2S3<L> THERMODATA 01/86 BC
TRITHIO-CARBONIC ACID. Liquid Standard State.
C1H4O1<L> I. BARIN 3rd. Edition
C1H4O1 CH3OH
METHANOL. H298 and S298 modified.
C1H4S1<L> THERMODATA 04/99 HH
METHANETHIOL. Liquid Standard State.
C1H4<L> THERMODATA 04/99 HH
METHANE Liquid Standard State.
C1S2<L> KUBASCHEWSKI EVANS ALCOCK 1967 SGTE
C1S2 CS2
CARBON DISULFIDE
C1S2 MELTS AT 161.15K LF=1.05(0.1)KCAL/MOLE
C2H4O2<L> THERMODATA 01/93
C2H4O2
ACETIC ACID
28/01/93 Tb=389K.
C2H6O1<L> THERMODATA 01/93
C2H6O1 C2H6O
ETHANOL
28/01/93
C2H6O2<L> THERMODATA
C2H6O2
E-GLYCOL
Data revised by THDA.
C2H6<L> THERMODATA 04/99 HH
ETHANE Liquid Standard State.
C3H6<L> THERMODATA 03/05 HH
CYCLOPROPANE. Liquid Standard State.
C3H8<L> THERMODATA 04/99 HH
PROPANE Liquid Standard State
C4H8<L> THERMODATA 04/99 HH
CYCLOBUTANE. Liquid Standard State.
C60 MHR-95
C60
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.
The
Fitted to the data in [94Kor/Sid], who took the phase transition at
257K
that [94Kor/Sid] do not give an explicit value for S(298.15K).
S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =425.8 and Cp
e
calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]
in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.
Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
the value preferred, if obliquely, by [94Kor/Sid].
[92Ste/Chi]W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,
P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).
C6H6<L> THERMODATA 04/99 BC
BENZENE. Liquid Standard State. Tm=278.6K
C1 S.G.T.E. **
GRAPHITE
Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
C1<DIAMOND> S.G.T.E. **
C1<DIAMOND> <DIAMOND>
DIAMOND
Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
from 1994 database (ex THERMODATA 01/93)
H10O8S1<L> THERMODATA 01/93
H10O8S1

```
      SULFURIC ACID TETRAHYDRATE.
      28/01/93
   H15O10.5S1<L> THERMODATA 01/93
      H15O10.5S1
      SULFURIC ACID HEMIHEXAHYDRATE.
      28/01/93
   H2O1<L> T.C.R.A.S. Class: 4
      H2O1 H2O
      WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002
   H2O2<L> THERMODATA 01/93
      H2O2 H2O2
      HYDROGEN PEROXIDE
      28/01/93
   H2O4S1<L> THERMODATA 01/93
      H2O4S1 H2SO4
      SULFURIC ACID
      28/01/93 Tb = 553K.
      S298 modified by NPL 24/11/94. Negative value in Thermodata.
   H2S1<L> THERMODATA 12/94 KK
      HYDROGEN SULFIDE. Liquid Standard State.
   H2S2<L> THERMODATA 11/99 KK
      Liquid standard State.
   H4O5S1<L> THERMODATA 01/93
      H4O5S1
      SULFURIC ACID MONOHYDRATE.
      28/01/93
   H6O6S1<L> THERMODATA 01/93
      H6O6S1
      H2SO4-2H2O
      28/01/93
   H8O7S1<L> Janaf 4th. Edition
      H8O7S1 H2SO4.3H2O
      SULFURIC ACID TRIHYDRATE
   O3S1<L> THERMODATA 12/94 KK
      SULFUR OXIDE BETA. Liquid Standard State.
   S1 T.C.R.A.S Class: 5
      S1
      Data provided by T.C.R.A.S. October 1994.
      Data refitted by I.A.
 -OK-
TDB_SSUB6: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: 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: s-i-a n(h2)=10
   ... the command in full is SET_INPUT_AMOUNTS
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 N(H)=20
 DEGREES OF FREEDOM 5
POLY: s-i-a n(c1o2)=5
   ... the command in full is SET_INPUT_AMOUNTS
POLY: s-i-a n(o2s1)=0.1
   ... the command in full is SET_INPUT_AMOUNTS
POLY: 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: s-c t=1000 p=1e5
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           132 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB6

 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  H1O1S1_SOH    3.35036E-14  C4H8_6        1.82465E-21
 H2O1          2.15350E-01  C2H6O1_1      2.75193E-14  O2            1.79235E-21
 C1O1          1.95778E-01  C2H5          2.60816E-14  C2O1          1.66878E-21
 C1O2          1.36417E-01  C3H8          1.55219E-14  S5            8.95084E-22
 H2S1          6.57218E-03  C1H3O1_CH2OH  7.69302E-15  C2H2O1        5.16353E-22
 C1H4          3.01187E-03  H2O1S1_H2SO   2.59570E-15  C4H6_5        3.26857E-22
 C1O1S1        1.34465E-04  C2H3          1.30277E-15  C3H6O1_2      9.94895E-23
 H1S1          5.08063E-08  C3H4_2        1.28184E-15  C4H8_4        5.15316E-23
 C1H2O1        4.89873E-08  C3O2          7.11139E-16  H2O4S1        1.59729E-23
 C1H2O2_CIS    4.46604E-08  C3H4_1        3.44164E-16  C4H2_1        8.50232E-24
 H2S2          3.75745E-08  H1O1S1_HSO    1.08974E-16  C4H2_2        8.48033E-24
 C1S2          1.41821E-08  C3H6_1        5.22179E-17  C6H6O1        6.55562E-24
 S2            1.10500E-08  C1H3O1_CH3O   1.80849E-17  H1O2          1.72311E-24
 C1H2O2_TRANS  6.42811E-09  C2H6O1_2      9.96672E-18  C2H1          3.18714E-25
 C2H6          3.64609E-09  C2H4O1_OXIRA  2.11511E-18  S6            2.65463E-26
```

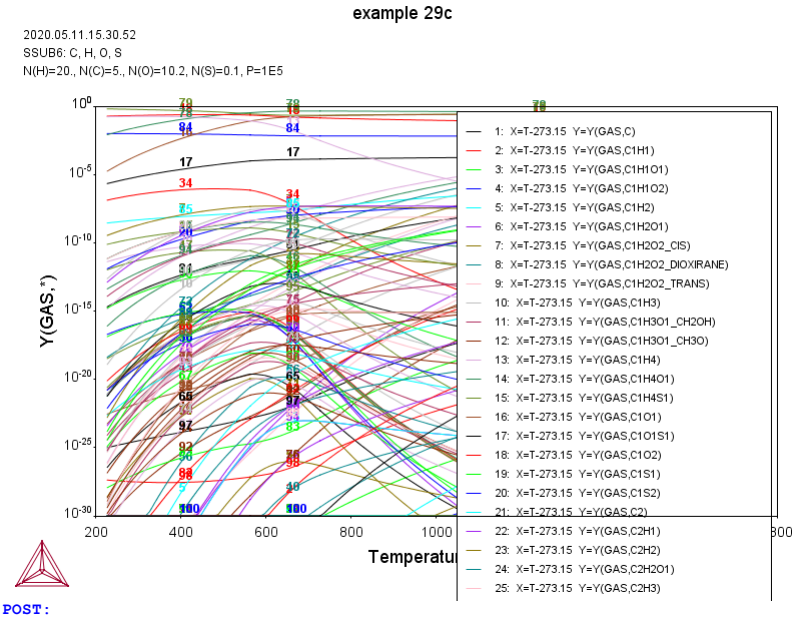
```
 C2H4           3.02667E-09  C4H6_2         1.29360E-18  C1H1           5.08634E-27
 H              1.51148E-09  S4             1.12104E-18  C4H4_1         4.75003E-27
 C1H4O1         1.14083E-09  C4H8_5         6.89221E-19  C3H1           9.91558E-28
 O2S1           2.26895E-10  C4H8_1         5.18832E-19  C1H2O2_DIOXI   4.40433E-30
 C1H3           1.88514E-10  C4H8_2         4.53214E-19  C              1.00000E-30
 C1H4S1         1.76437E-10  C4H8_3         3.93010E-19  C2             1.00000E-30
 H2O1S1_HSOH    8.67082E-11  C3H6O1_1       2.60648E-19  C2H4O2_DIOXE   1.00000E-30
 C2H4O1_ACETA   2.61120E-11  C2H6O2         2.59417E-19  C2H4O3_123TR   1.00000E-30
 C2H2           1.43254E-11  C1H2           2.13894E-19  C2H4O3_124TR   1.00000E-30
 O1S1           1.05406E-11  C4H10_1        8.31953E-20  C3             1.00000E-30
 C1H1O1         9.19785E-12  C4H10_2        4.22679E-20  C4             1.00000E-30
 C1S1           5.40802E-12  C6H6           3.95182E-20  C4H1           1.00000E-30
 C2H4O2_ACETI   4.53120E-12  H2O2           2.47048E-20  C5             1.00000E-30
 H1O1           1.61961E-12  C4H6_4         1.91129E-20  C60            1.00000E-30
 O1S2           9.69426E-13  O3S1           1.73550E-20  O3             1.00000E-30
 C1H1O2         9.05180E-13  C4H6_1         1.14077E-20  S7             1.00000E-30
 S              7.19264E-13  O              6.65398E-21  S8             1.00000E-30
 S3             1.46179E-13  C4H6_3         6.48690E-21
 C3H6_2         1.11399E-13  C4H4_2         3.35580E-21
POLY:Hit RETURN to continue
POLY: s-a-v 1 t 500 2000 50
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex29 y
   ... the command in full is SAVE_WORKSPACES
POLY:

POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    1000.00
...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: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex29\tcex29.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST: @@ Plot the 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:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



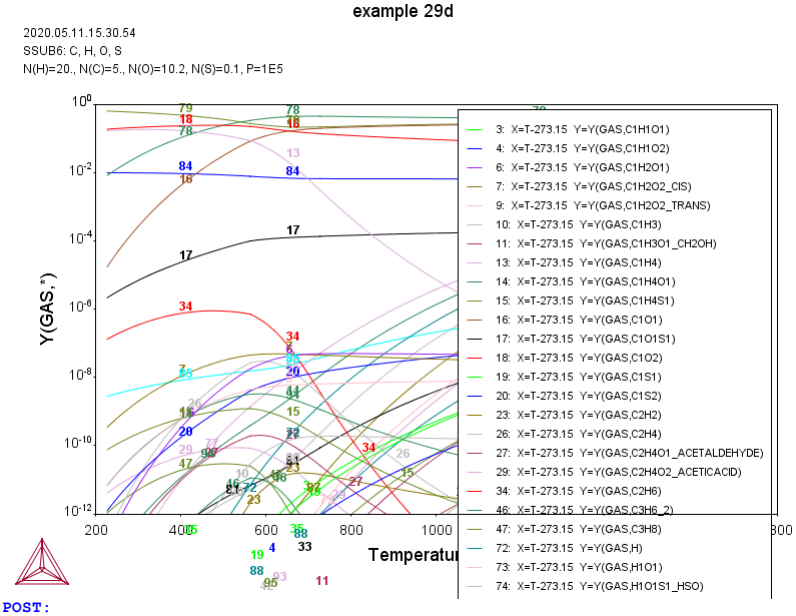

```
POST:
POST:Hit RETURN to continue
POST: @@ Plot gas speciation. y(gas,*) are partial
POST: @@ pressures expressed in bar (as total pressure
POST: @@ is one bar). Set labels on the lines.
POST: s-d-a y y(gas,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 29b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Set a logarithmic axis
POST: s-ax-ty
   ... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : y
AXIS TYPE /LINEAR/: log
POST:
POST: set-title example 29c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Set scaling
POST: s-s y n 1e-12 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 29d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



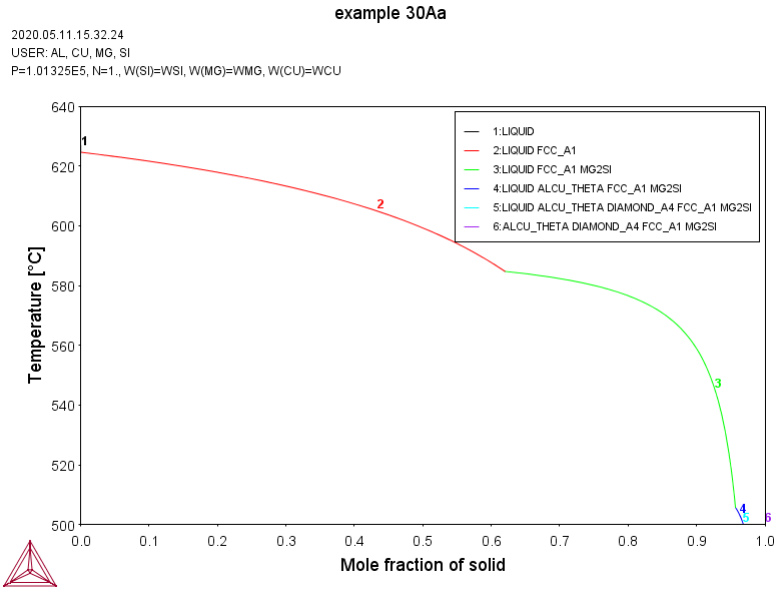

```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex30A

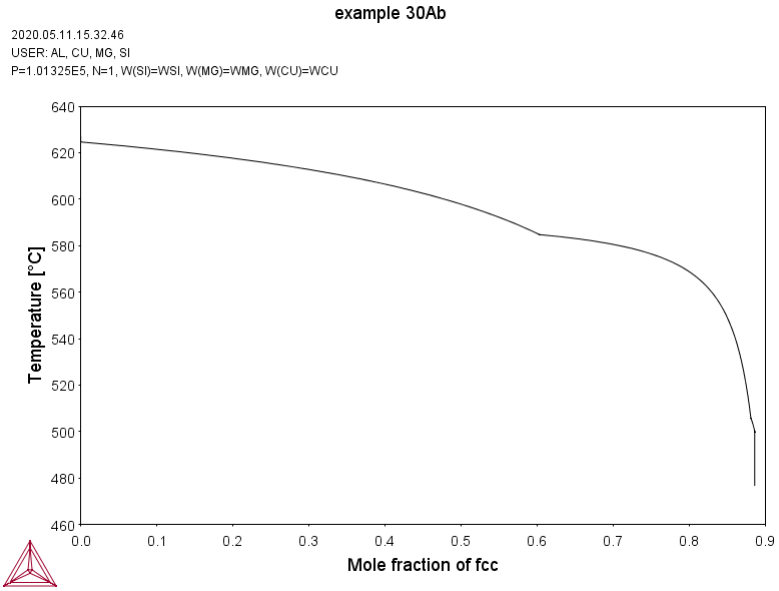
```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex30A\tcex30A.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Scheil calculation for an Al-4Mg-2Si-2Cu alloy
SYS:
SYS: @@ This is the first of two examples showing how to
SYS: @@ do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy.
SYS: @@ In part A, you use the POLY3 module and the
SYS: @@ STEP_WITH_OPTIONS command with an EVALUATE setting.
SYS: @@ Then in part B you use the SCHEIL module commands to
SYS: @@ do the same thing.
SYS:
SYS: go da
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw user tcex30_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                      /-  DEFINED
15:32:11,462 INFO  USER_199218156_11, number of lines read: 880
15:32:12,036 INFO  Parsing of USER_199218156_11 completed in 667 ms
TDB_USER: def-ele al cu mg si
 AL                      CU                      MG
 SI  DEFINED
TDB_USER: get
15:32:12,177 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
  'COST (1998): COST 507 -- Definition of Thermochemical and Thermophysical
      Properties to Provide a Database for the Development of New Light
      Alloys. European Cooperation in the Field of Scientific and Technical
      Research, European Commission. Vol 1. Proceedings of the Final
      Workshop of COST 507, Vaals, the Netherlands, 1997; Vol 2.
      Thermochemical Database for Light Metal Alloys (Eds. Ansara I.,
      Dinsdale A.T., and Rand M.H.); Vol 3. Critical Evaluation of Ternary
      Systems (Ed. Effenberg G.). '
 -OK-
TDB_USER: go p-3

 POLY version  3.32
POLY: s-c p=101325 n=1 t=1000 w(si)=0.02 w(mg)=0.04 w(cu)=0.02
POLY: c-e
 Using global minimization procedure
15:32:13,160 INFO  Preparing system for use: USER_199218156_11
15:32:13,973 INFO  Preparing phase for use: LIQUID
15:32:14,248 INFO  Preparing phase for use: AL12MG17
15:32:14,441 INFO  Preparing phase for use: ALCE_AMORPHOUS
15:32:14,554 INFO  Preparing phase for use: ALCUZN_T
15:32:14,684 INFO  Preparing phase for use: ALCU_DELTA
15:32:14,780 INFO  Preparing phase for use: ALCU_EPSILON
15:32:14,937 INFO  Preparing phase for use: ALCU_ETA
15:32:15,054 INFO  Preparing phase for use: ALCU_PRIME
15:32:15,188 INFO  Preparing phase for use: ALCU_THETA
15:32:15,309 INFO  Preparing phase for use: ALCU_ZETA
15:32:15,405 INFO  Preparing phase for use: ALLI
15:32:15,546 INFO  Preparing phase for use: ALMG_BETA
15:32:15,670 INFO  Preparing phase for use: ALMG_EPS
15:32:15,844 INFO  Preparing phase for use: ALMG_GAMMA
15:32:15,944 INFO  Preparing phase for use: ALMO
15:32:16,040 INFO  Preparing phase for use: ALM_D019
15:32:16,140 INFO  Preparing phase for use: ALND_AMORPHOUS
15:32:16,263 INFO  Preparing phase for use: ALTI
15:32:16,404 INFO  Preparing phase for use: BCC_B2
15:32:16,497 INFO  Preparing phase for use: BCC_A2
15:32:16,681 INFO  Preparing phase for use: BCT_A5
15:32:16,780 INFO  Preparing phase for use: CBCC_A12
15:32:16,912 INFO  Preparing phase for use: CR3SI_A15
15:32:17,021 INFO  Preparing phase for use: CRSI2
15:32:17,108 INFO  Preparing phase for use: CU19SI6_ETA
15:32:17,245 INFO  Preparing phase for use: CU33SI7_DELTA
15:32:17,330 INFO  Preparing phase for use: CU4SI_EPSILON
15:32:17,419 INFO  Preparing phase for use: CU56SI11_GAMMA
15:32:17,511 INFO  Preparing phase for use: CU6Y
15:32:17,606 INFO  Preparing phase for use: CUB_A13
15:32:17,711 INFO  Preparing phase for use: CUB_A15
15:32:17,809 INFO  Preparing phase for use: CUMG2
15:32:17,915 INFO  Preparing phase for use: CUMGSI_SIGMA
15:32:18,004 INFO  Preparing phase for use: CUMGSI_TAU
15:32:18,087 INFO  Preparing phase for use: CUZN_GAMMA
15:32:18,179 INFO  Preparing phase for use: DIAMOND_A4
15:32:18,279 INFO  Preparing phase for use: FCC_A1
15:32:18,421 INFO  Preparing phase for use: GAMMA_D83
15:32:18,528 INFO  Preparing phase for use: GAMMA_H
15:32:18,619 INFO  Preparing phase for use: HCP_A3
15:32:18,754 INFO  Preparing phase for use: HCP_ZN
```

```
15:32:18,860 INFO  Preparing phase for use: LAVES_C14
15:32:18,982 INFO  Preparing phase for use: LAVES_C15
15:32:19,081 INFO  Preparing phase for use: LAVES_C36
15:32:19,174 INFO  Preparing phase for use: MG24Y5
15:32:19,255 INFO  Preparing phase for use: MG2SI
15:32:19,339 INFO  Preparing phase for use: MG2Y
15:32:19,419 INFO  Preparing phase for use: MG2ZN11
15:32:19,501 INFO  Preparing phase for use: MG2ZN3
15:32:19,624 INFO  Preparing phase for use: MGY_GAMMA
15:32:19,707 INFO  Preparing phase for use: MGZN
15:32:19,788 INFO  Preparing phase for use: PHI
15:32:19,888 INFO  Preparing phase for use: QPHASE
15:32:19,980 INFO  Preparing phase for use: SIV3
15:32:20,062 INFO  Preparing phase for use: SPHASE
15:32:20,234 INFO  Preparing phase for use: TAU
15:32:20,352 INFO  Preparing phase for use: VPHASE
Calculated         26538 grid points in            11 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time    12  s
POLY: 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: @@ calculate liquidus temperature in order to choose

POLY: @@  a starting temperature where only liquid exists
POLY: c-st phase fcc_a1=fix 0
POLY: s-c t=none
POLY: c-e
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         26538 grid points in             0 s
    12 ITS,  CPU TIME USED   0 SECONDS
POLY: 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: show t
 T=897.74074
POLY:Hit RETURN to continue
POLY: s-c t
Value /897.7407448/: 900
POLY: c-st phase
Phase name(s): fcc_a1
Status: /ENTERED/: ENTERED
Start value, number of mole formula units /0/: 0
POLY: c-e
 Using global minimization procedure
Calculated         26538 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: 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: s-a-v 1 t
Min value /0/: 750 900 1
POLY:
```

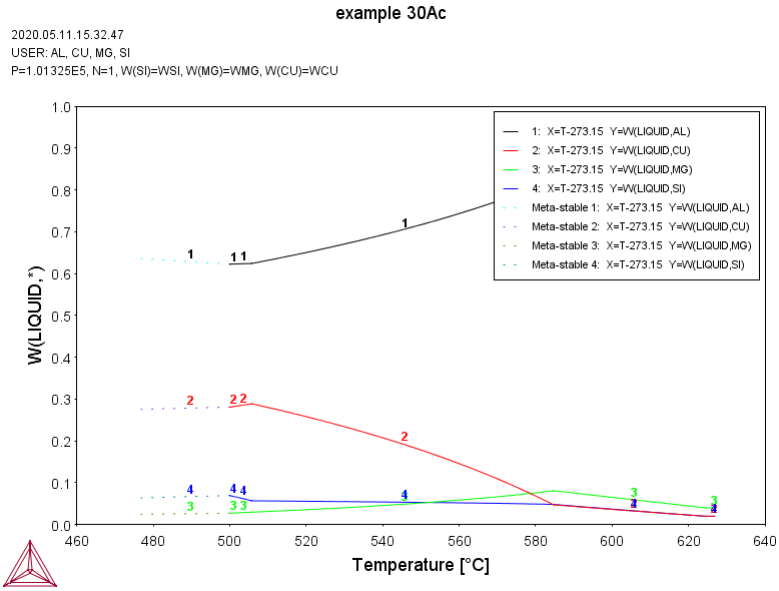
```
POLY: ent var nl=1;
POLY: ent var nfcc=0;
POLY: ent var nl=np(liquid)*nl;
POLY: ent fun ns=1-nl;
POLY: ent var nfcc=nfcc+nl*np(fcc_a1);
POLY: ent var wsi=w(liquid,si);
POLY: ent var wmg=w(liquid,mg);
POLY: ent var wcu=w(liquid,cu);
POLY: ent tab tab1
Variable(s): t nl ns nfcc
&
POLY: s-c w(si)=wsi w(mg)=wmg w(cu)=wcu
 Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
 Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
 Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
POLY: save tcex30a y
POLY:
POLY: step
Option? /NORMAL/: eva
Variable name(s): wsi wmg wcu
 No initial equilibrium, using default
...OK

 Phase Region from    900.000     for:
     LIQUID
 Global check of adding phase at  8.97741E+02
 Calculated     5 equilibria

 Phase Region from    897.741     for:
     LIQUID
     FCC_A1
 Global test at  8.90000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  8.70000E+02 .... OK
 Global test at  8.60000E+02 .... OK
 Global check of adding phase at  8.57875E+02
 Calculated    43 equilibria

 Phase Region from    857.875     for:
     LIQUID
     FCC_A1
     MG2SI
 Global test at  8.50000E+02 .... OK
 Global test at  8.40000E+02 .... OK
 Global test at  8.30000E+02 .... OK
 Global test at  8.20000E+02 .... OK
 Global test at  8.10000E+02 .... OK
 Global test at  8.00000E+02 .... OK
 Global test at  7.90000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global check of adding phase at  7.78888E+02
 Calculated    82 equilibria

 Phase Region from    778.888     for:
     LIQUID
     ALCU_THETA
     FCC_A1
     MG2SI
 Global check of adding phase at  7.73208E+02
 Calculated     8 equilibria

 Phase Region from    773.208     for:
     LIQUID
     ALCU_THETA
     DIAMOND_A4
     FCC_A1
     MG2SI
 Calculated     2 equilibria

 Phase Region from    773.208     for:
     ALCU_THETA
     DIAMOND_A4
     FCC_A1
     MG2SI
 Global test at  7.66000E+02 .... OK
 Global test at  7.56000E+02 .... OK
 Terminating at    750.000
 Calculated    27 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex30A\tcex30a.POLY3
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x tab1
COLUMN NUMBER /*/: 3
POST: s-d-a y t-c
POST:
POST: s-s-s y
AUTOMATIC SCALING  (Y OR N) /N/: n
MIN VALUE : 500 640
POST: s-lab b
POST: se-ax-te x n
AXIS TEXT : Mole fraction of solid
POST: set-title example 30Aa
POST: plot
```




```
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST:
POST:Hit RETURN to continue
POST: back
POLY: read,,
POLY: po
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x tab1
COLUMN NUMBER /*/: 4
POST: s-d-a y t-c
POST: se-ax-te x n
AXIS TEXT : Mole fraction of fcc
POST: set-title example 30Ab
POST:
POST: plot
```




```
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST:
POST:Hit RETURN to continue
POST: s-d-a x t-c
POST: s-d-a y w(liquid,*),,
POST: set-title example 30Ac
POST: s-l d
POST:
POST: plot
```




```
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST:
POST: set-inter
POST:
```

tcex30B

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex30B\tcex30B.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Scheil calculation for an Al-4Mg-2Si-2Cu alloy
SYS:
SYS: @@ This is the second of two examples showing how to
SYS: @@ do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy.
SYS: @@ In part A, you used the POLY3 module and the
SYS: @@ STEP_WITH_OPTIONS command with an Evaluate setting.
SYS:
SYS: @@ This is part B where you use the SCHEIL module commands
SYS: @@ to do the same thing.
SYS:
SYS: go scheil
SCHEIL: start
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: user tcex30_cost2.TDB
 Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

 VA                       /-  DEFINED
15:34:06,977 INFO  USER_1196290509_11, number of lines read: 880
15:34:07,557 INFO  Parsing of USER_1196290509_11 completed in 681 ms
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 GES .....
 AL  DEFINED
 MG  DEFINED
 SI  DEFINED
 CU  DEFINED


 This database has following phases for the defined system

 LIQUID:L                 AL12MG17                 ALCE_AMORPHOUS
 ALCUZN_T                 ALCU_DELTA               ALCU_EPSILON
 ALCU_ETA                 ALCU_PRIME               ALCU_THETA
 ALCU_ZETA                ALLI                     ALMG_BETA
 ALMG_EPS                 ALMG_GAMMA               ALMO
 ALM_D019                 ALND_AMORPHOUS           ALTI
 BCC_A2                   BCC_B2                   BCT_A5
 CBCC_A12                 CR3SI_A15                CRSI2
 CU19SI6_ETA              CU33SI7_DELTA            CU4SI_EPSILON
 CU56SI11_GAMMA           CU6Y                     CUB_A13
 CUB_A15                  CUMG2                    CUMGSI_SIGMA
 CUMGSI_TAU               CUZN_GAMMA               DIAMOND_A4
 FCC_A1                   GAMMA_D83                GAMMA_H
 HCP_A3                   HCP_ZN                   LAVES_C14
 LAVES_C15                LAVES_C36                MG24Y5
 MG2SI                    MG2Y                     MG2ZN11
 MG2ZN3                   MGY_GAMMA                MGZN
 PHI                      QPHASE                   SIV3
 SPHASE                   TAU                      VPHASE
Reject phase(s) /NONE/: *
 LIQUID:L                 AL12MG17                 ALCE_AMORPHOUS
 ALCUZN_T                 ALCU_DELTA               ALCU_EPSILON
 ALCU_ETA                 ALCU_PRIME               ALCU_THETA
 ALCU_ZETA                ALLI                     ALMG_BETA
 ALMG_EPS                 ALMG_GAMMA               ALMO
 ALM_D019                 ALND_AMORPHOUS           ALTI
 BCC_A2                   BCC_B2                   BCT_A5
 CBCC_A12                 CR3SI_A15                CRSI2
 CU19SI6_ETA              CU33SI7_DELTA            CU4SI_EPSILON
 CU56SI11_GAMMA           CU6Y                     CUB_A13
 CUB_A15                  CUMG2                    CUMGSI_SIGMA
 CUMGSI_TAU               CUZN_GAMMA               DIAMOND_A4
 FCC_A1                   GAMMA_D83                GAMMA_H
 HCP_A3                   HCP_ZN                   LAVES_C14
 LAVES_C15                LAVES_C36                MG24Y5
 MG2SI                    MG2Y                     MG2ZN11
 MG2ZN3                   MGY_GAMMA                MGZN
 PHI                      QPHASE                   SIV3
 SPHASE                   TAU                      VPHASE
   REJECTED
Restore phase(s):: liquid fcc_a1 alcu_th mg2si diamond_a4 al12mg17
 LIQUID:L                 FCC_A1                   ALCU_THETA
 MG2SI                    DIAMOND_A4               AL12MG17
   RESTORED
Restore phase(s): /NONE/:

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

    The following phases are retained in this system:

 LIQUID:L                 AL12MG17                 ALCU_THETA
 DIAMOND_A4               FCC_A1                   MG2SI

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

```
OK? /Y/: Y
 *** ERROR GAS INPUT IGNORED
15:34:07,711 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
      1999/2003. '
  'COST (1998): COST 507 -- Definition of Thermochemical and Thermophysical
      Properties to Provide a Database for the Development of New Light
      Alloys. European Cooperation in the Field of Scientific and Technical
      Research, European Commission. Vol 1. Proceedings of the Final
      Workshop of COST 507, Vaals, the Netherlands, 1997; Vol 2.
      Thermochemical Database for Light Metal Alloys (Eds. Ansara I.,
      Dinsdale A.T., and Rand M.H.); Vol 3. Critical Evaluation of Ternary
      Systems (Ed. Effenberg G.). '
 -OK-
Should any phase have a miscibility gap check? /N/: N
15:34:08,632 INFO  Preparing system for use: USER_1196290509_11
15:34:09,341 INFO  Preparing phase for use: LIQUID
15:34:09,627 INFO  Preparing phase for use: AL12MG17
15:34:09,791 INFO  Preparing phase for use: ALCU_THETA
15:34:09,909 INFO  Preparing phase for use: DIAMOND_A4
15:34:10,108 INFO  Preparing phase for use: FCC_A1
15:34:10,266 INFO  Preparing phase for use: MG2SI
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/:
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=1073.15, W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0
 PHASE CHANGE AT 897.740742588
FCC_A1#1 forms
 Testing POLY result by global minimization procedure
Calculated          5945 grid points in           0 s
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

 Phase Region from    897.831     for:
     LIQUID
 Terminating at    897.931
 Calculated     4 equilibria

 Phase Region from    897.831     for:
     LIQUID
 Global check of adding phase at  8.97741E+02
 Calculated     3 equilibria

 Phase Region from    897.741     for:
     LIQUID
     FCC_A1
 Global test at  8.89831E+02 .... OK
 Global test at  8.79831E+02 .... OK
 Global test at  8.69831E+02 .... OK
 Global test at  8.59831E+02 .... OK
 Global check of adding phase at  8.57535E+02
 Calculated    43 equilibria

 Phase Region from    857.535     for:
     LIQUID
     FCC_A1
     MG2SI
 Global test at  8.49831E+02 .... OK
 Global test at  8.39831E+02 .... OK
 Global test at  8.29831E+02 .... OK
 Global check of removing phase at  8.26196E+02
 Calculated    34 equilibria

 Phase Region from    826.196     for:
     FCC_A1
     MG2SI
 Calculated     4 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\SCHEIL_2356.POLY3
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

 An EXP file C:\Users\vagrant\AppData\Local\Temp\SCHEIL_EQ_2356.EXP
 has been created to store the equilibrium solidification results.
  CALCULATING SCHEIL SOLIDFICATION
     T(C)      fraction solid
   624.6807       0.000000
 PHASE REGION:LIQUID + FCC_A1
     T(C)      fraction solid
   624.5851      0.2038889E-03
   623.5851      0.3538798E-01
   622.5851      0.6842453E-01
   621.5851      0.9949709E-01
   620.5851      0.1287693
   619.5851      0.1563873
   618.5851      0.1824824
   617.5851      0.2071723
   616.5851      0.2305634
   615.5851      0.2527515
   614.5851      0.2738237
   613.5851      0.2938587
   612.5851      0.3129285
   611.5851      0.3310983
   610.5851      0.3484280
   609.5851      0.3649722
   608.5851      0.3807809
   607.5851      0.3959003
   606.5851      0.4103725
   605.5851      0.4242366
   604.5851      0.4375286
```

603.5851	0.4502817
602.5851	0.4625266
601.5851	0.4742918
600.5851	0.4856038
599.5851	0.4964872
598.5851	0.5069647
597.5851	0.5170577
596.5851	0.5267860
595.5851	0.5361681
594.5851	0.5452213
593.5851	0.5539619
592.5851	0.5624050
591.5851	0.5705648
590.5851	0.5784547
589.5851	0.5860871
588.5851	0.5934739
587.5851	0.6006261
586.5851	0.6075542
585.5851	0.6142679

PHASE REGION:LIQUID + FCC_A1 + MG2SI

T(C)	fraction solid
584.7245	0.6199090
583.7245	0.6576760
582.7245	0.6886411
581.7245	0.7144754
580.7245	0.7363465
579.7245	0.7550939
578.7245	0.7713365
577.7245	0.7855406
576.7245	0.7980640
575.7245	0.8091857
574.7245	0.8191265
573.7245	0.8280633
572.7245	0.8361395
571.7245	0.8434725
570.7245	0.8501596
569.7245	0.8562816
568.7245	0.8619067
567.7245	0.8670925
566.7245	0.8718879
565.7245	0.8763351
564.7245	0.8804703
563.7245	0.8843250
562.7245	0.8879265
561.7245	0.8912987
560.7245	0.8944628
559.7245	0.8974371
558.7245	0.9002382
557.7245	0.9028806
556.7245	0.9053773
555.7245	0.9077400
554.7245	0.9099790
553.7245	0.9121039
552.7245	0.9141230
551.7245	0.9160440
550.7245	0.9178738
549.7245	0.9196187
548.7245	0.9212845
547.7245	0.9228765
546.7245	0.9243993
545.7245	0.9258573
544.7245	0.9272547
543.7245	0.9285951
542.7245	0.9298819
541.7245	0.9311183
540.7245	0.9323071
539.7245	0.9334511
538.7245	0.9345527
537.7245	0.9356142
536.7245	0.9366378
535.7245	0.9376256
534.7245	0.9385793
533.7245	0.9395007
532.7245	0.9403914
531.7245	0.9412529
530.7245	0.9420867
529.7245	0.9428941
528.7245	0.9436762
527.7245	0.9444344
526.7245	0.9451697
525.7245	0.9458831
524.7245	0.9465756
523.7245	0.9472482
522.7245	0.9479016
521.7245	0.9485367
520.7245	0.9491543
519.7245	0.9497551
518.7245	0.9503399
517.7245	0.9509091
516.7245	0.9514636
515.7245	0.9520038
514.7245	0.9525303
513.7245	0.9530437
512.7245	0.9535444
511.7245	0.9540330
510.7245	0.9545099
509.7245	0.9549755
508.7245	0.9554302
507.7245	0.9558745
506.7245	0.9563086

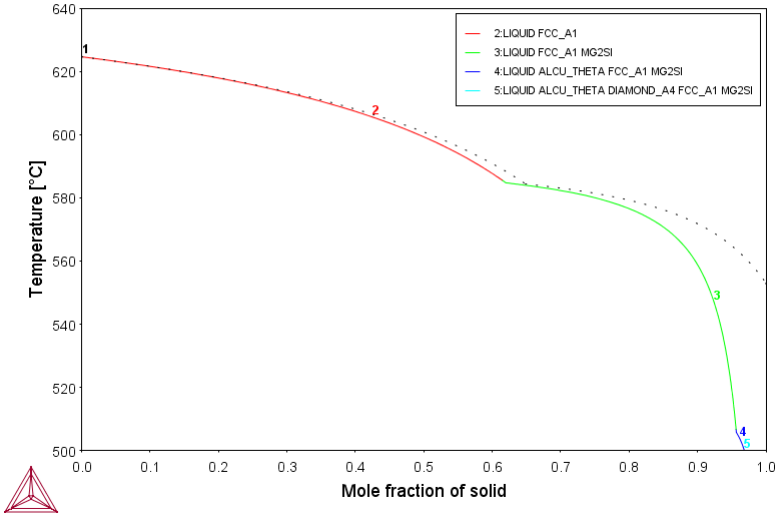
PHASE REGION:LIQUID + ALCU_THETA + FCC_A1 + MG2SI

T(C)	fraction solid
505.7364	0.9567319
504.7364	0.9594803
503.7364	0.9618348
502.7364	0.9638799
501.7364	0.9656767
500.7364	0.9672706
500.0670	0.9682413

PHASE REGION:ALCU_THETA + DIAMOND_A4 + FCC_A1 + MG2SI

T(C)	fraction solid
500.0351	1.000000

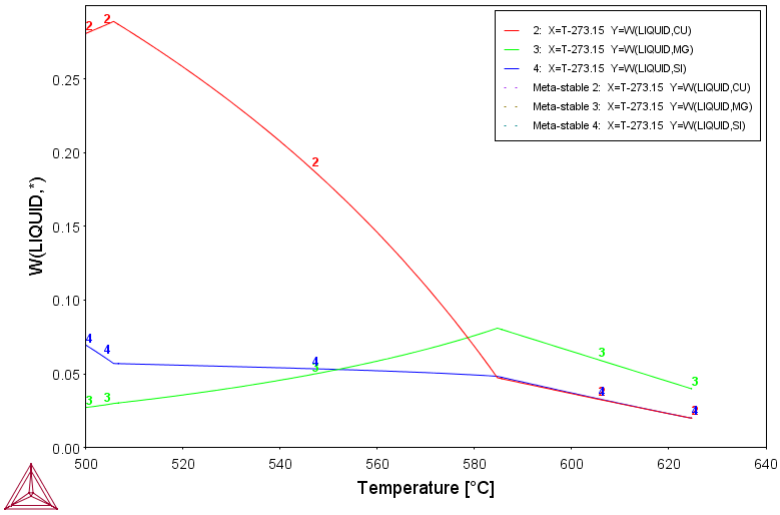
2020.05.11.15.34.12
USER: AL, CU, MG, SI
T=897.831, W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=1E5, N=1




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

        The following axis variables are available

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

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

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

```
POST:
POST:Hit RETURN to continue
POST: s-d-a x t
POST: s-d-a y w(liquid,*),,,,,,
POST: s-s-s y n 0 0.3
POST: set-lab F
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,,
```

2020.05.11.15.34.36
USER: AL, CU, MG, SI
T=897.831, W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=1E5, N=1




```
POST:
POST: set-inter
POST:
```

tcex31

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex31\tcex31.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Using the GESÂ module to calculate CVM
SYS:
SYS: @@ This example calculates the CVM and compares it with the
SYS: @@ sublattices of a fictitious A B system. You also learn how
SYS: @@ to overlay diagrams from two calculations.
SYS:
SYS: @@ This example uses some GES commands that are not yet
SYS: @@ supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: set-log ex31,,,
SYS:
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
GES:
GES: @@ Enter the elements and the reference states
GES: e-e A B
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 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
GES: @@ needed as the B atom can be on 4 different sublattices etc.
GES:
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
GES: @@ 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
GES: @@ A3B, A2B2 and AB3 respectivly.
GES: @@ In the simplest case, like here, they are just the
GES: @@ bond energy multiplied with 3, 4 and 3, respectively.
GES:
```

```
GES: e-sy fun GA3B1,,3*UIJ;,,,
   ... the command in full is ENTER_SYMBOL
GES: e-sy fun GA2B2,,4*UIJ;,,,
   ... the command in full is ENTER_SYMBOL
GES: e-sy fun GA1B3,,3*UIJ;,,,
   ... the command in full is ENTER_SYMBOL
GES:
GES: @@ ==================================================
GES: @@ This is the FCC phase with CVM for both LRO and SRO
GES: e-ph CVM_TET
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S4
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES: E-PAR G(C,S11),,GA3B1;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(C,S12),,GA3B1;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(C,S13),,GA3B1;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(C,S14),,GA3B1;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(C,S21),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S22),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S23),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S24),,GA2B2;,,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S25),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S26),,GA2B2;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: E-PAR G(C,S31),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(C,S32),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(C,S33),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: E-PAR G(C,S34),,GA1B3;,,,
   ... the command in full is ENTER_PARAMETER
 G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0)
GES: l-d,,,,
   ... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

 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
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   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:
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: @@ parameter is simply 12 times the bond energy as the ;1 and ;2
GES: @@ parameters cancel when GA1B3=GA3B1=0.75*GA2B2
GES:
GES: e-ph fcc_a1
   ... the command in full is ENTER_PHASE
TYPE CODE:
```

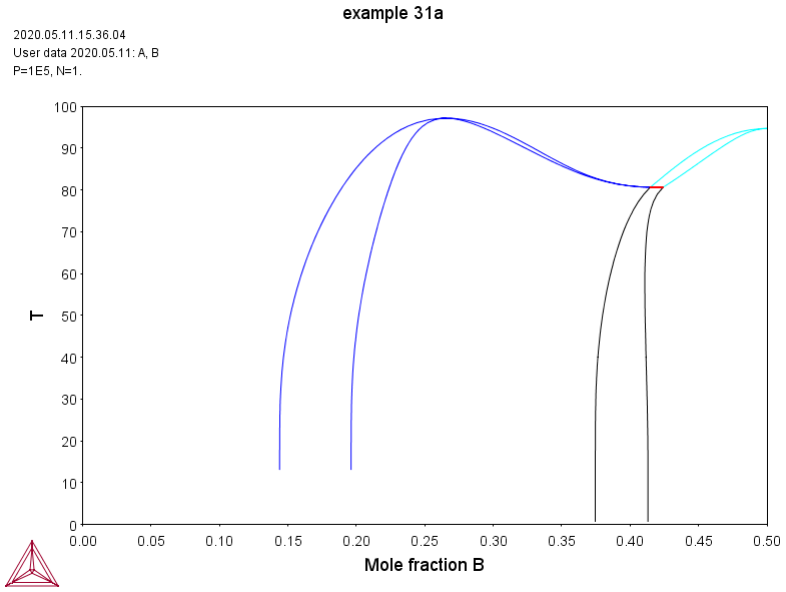
```
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES:
GES: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3;,,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B;0)
GES: e-par 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, add together the LRO phase with the disordered FCC
GES: @@ Note that the parameters in LRO give zero contribution
GES: @@ when the phase is disordered
GES:
GES: amend-phase LRO dis FCC
   ... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: @@
GES: @@ This is the 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
 Creating a new composition set CVM_TET#2
 GIVE FOR COMPOSITION SET                    2
Major constituent(s) for sublattice 1: /$/: s11
 Creating a new composition set CVM_TET#2
 GIVE FOR COMPOSITION SET                    3
Major constituent(s) for sublattice 1: /$/: 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
 Creating a new composition set LRO#2
 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/: *
 Creating a new composition set LRO#2
 GIVE FOR COMPOSITION SET                    3
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: B
Major constituent(s) for sublattice 4: /A B/: B
GES: am-ph lro
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: maj
Composition set /1/: 1
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: A
Major constituent(s) for sublattice 4: /A B/: B
GES:
GES: l-d,,,,
   ... the command in full is LIST_DATA
```

```
1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

 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
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   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 start the calculation
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:

POLY: @@ Turn global minimization off
POLY: 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:
POLY: L-C
   ... the command in full is LIST_CONDITIONS
 DEGREES OF FREEDOM 4
POLY: S-C T=60 P=1E5 N=1 X(B)=.4
   ... the command in full is SET_CONDITION
POLY: @@
POLY: @@ First calculate just with the full CVM phases
POLY: ch-st ph *=sus
   ... the command in full is CHANGE_STATUS
POLY: ch-st ph cvm cvm#2 cvm#3=ent 1
   ... the command in full is CHANGE_STATUS
POLY: @@
POLY: @@ L10 ordering, setting start composition essential
POLY: @@ The initial fraction of each species is bascially
POLY: @@ calculated as the product of the site fraction on
POLY: @@ each sublattice.
POLY: 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:
POLY: @@ L12 ordering
POLY: 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:
POLY: s-s-c cvm#3 *
   ... the command in full is SET_START_CONSTITUTION
POLY:
POLY: 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xnp
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=60, P=1E5, N=1, X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     60.00 K (  -213.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.10213E+03,  Enthalpy -2.96850E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 2.0465E-02 -1.9401E+03 SER
 B                       4.0000E-01  4.0000E-01 6.0538E-05 -4.8452E+03 SER

 CVM_TET#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  S21  1.28068E-02  S33  4.13398E-03  S22  2.56479E-04
 S12  1.76120E-01  S23  1.28068E-02  S0   3.76373E-03  S34  1.15932E-04
 S14  1.76120E-01  S26  1.28068E-02  S13  2.78465E-03  S32  1.15932E-04
 S24  1.28068E-02  S31  4.13398E-03  S11  2.78465E-03  S4   3.67798E-06

 CVM_TET#2                   Status ENTERED     Driving force  0.0000E+00
 Moles 4.3050E-01, Mass 4.3050E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.14278E-01  B  3.85722E-01
 Constitution:
 S11  4.21306E-01  S14  1.38900E-02  S32  4.69234E-03  S25  3.19866E-03
 S22  1.69717E-01  S13  1.38900E-02  S34  4.69234E-03  S24  3.19866E-03
 S23  1.69717E-01  S12  1.38900E-02  S0   4.13973E-03  S31  5.05554E-05
 S21  1.69717E-01  S33  4.69234E-03  S26  3.19866E-03  S4   8.90403E-06

 CVM_TET#3                   Status ENTERED     Driving force -1.0709E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.09450E-01  B  3.90550E-01
 Constitution:
 S13  1.09230E-01  S22  8.47466E-02  S24  8.47466E-02  S32  8.87560E-03
 S14  1.09230E-01  S26  8.47466E-02  S21  8.47466E-02  S34  8.87560E-03
 S12  1.09230E-01  S23  8.47466E-02  S0   1.86436E-02  S33  8.87560E-03
 S11  1.09230E-01  S25  8.47466E-02  S31  8.87560E-03  S4   4.53364E-04
POLY:Hit RETURN to continue
```

```
POLY: s-c t=40
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    18 ITS,  CPU TIME USED   0 SECONDS
POLY: s-s-c cvm#3 *
   ... the command in full is SET_START_CONSTITUTION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    18 ITS,  CPU TIME USED   0 SECONDS
POLY: L-E
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNP/:
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=40, P=1E5, N=1, X(B)=0.4
 DEGREES OF FREEDOM 0

 Temperature     40.00 K (  -233.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.06232E+03,  Enthalpy -2.98938E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 4.1519E-03 -1.8239E+03 SER
 B                       4.0000E-01  4.0000E-01 3.7621E-07 -4.9199E+03 SER

 CVM_TET#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  S21  4.57470E-03  S31  6.44301E-04  S22  1.02379E-05
 S12  1.76201E-01  S23  4.57470E-03  S33  6.44301E-04  S34  4.02672E-06
 S14  1.76201E-01  S26  4.57470E-03  S11  4.60814E-04  S32  4.02672E-06
 S24  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  S24  4.03145E-04
 S22  1.66859E-01  S12  4.56422E-03  S32  7.57611E-04  S26  4.03145E-04
 S21  1.66859E-01  S13  4.56422E-03  S0   6.77145E-04  S31  4.66624E-07
 S23  1.66859E-01  S34  7.57611E-04  S25  4.03145E-04  S4   4.50770E-08

 CVM_TET#3                   Status ENTERED     Driving force -3.4466E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.15550E-01  B  3.84450E-01
 Constitution:
 S12  1.12327E-01  S21  8.23389E-02  S26  8.23389E-02  S33  8.17828E-03
 S13  1.12327E-01  S25  8.23389E-02  S22  8.23389E-02  S34  8.17828E-03
 S11  1.12327E-01  S23  8.23389E-02  S0   2.33728E-02  S32  8.17828E-03
 S14  1.12327E-01  S24  8.23389E-02  S31  8.17828E-03  S4   5.71422E-04
POLY:Hit RETURN to continue
POLY: s-a-v 1 x(b) 0 .5,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 t 0 100,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex31a y
   ... the command in full is SAVE_WORKSPACES
POLY: 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:
 c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex31\tcex3
 1a.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: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex31\tcex31a.POLY3
 CPU time for mapping                     1 seconds
POLY: po
   ... the command in full is POST
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x m-f b
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 0.5
   ... the command in full is SET_SCALING_STATUS
```

```
POST: s-s-s y n 0 100
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 31a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

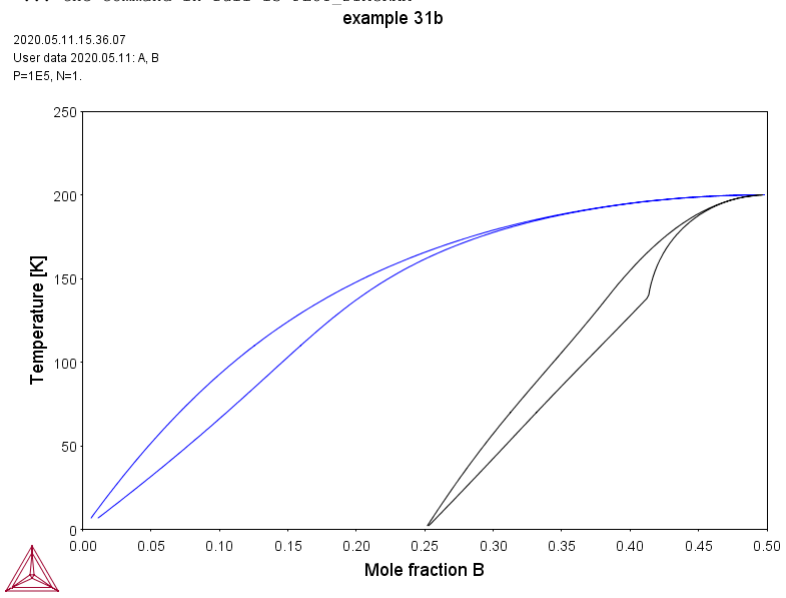



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Make an Experimental data file to overlay the next
POST: @@ calculation
POST: make tcex31 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY: @@
POLY: @@ It is interesting to compare with a CEF without any
POLY: @@ SRO contribution. This is the classical FCC ordering
POLY: @@ diagram first calculated manually by W Shockley,
POLY: @@ J Chem Phys, 6, (1938) p 130.
POLY: read tcex31a
   ... the command in full is READ_WORKSPACES
POLY: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:
POLY:Hit RETURN to continue
POLY: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY: c-st p lro lro#2 lro#3=ent 0
   ... the command in full is CHANGE_STATUS
POLY: s-c t=70 x(b)=.4
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    32 ITS,  CPU TIME USED   0 SECONDS
POLY: 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                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 2.6762E-01, Mass 2.6762E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.74559E-01  B  3.25441E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.99309E-01  B  1.00691E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99692E-01  A  3.08116E-04

 LRO#2                    DISORD Status ENTERED   Driving force -4.6485E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.45965E-01  B  3.54035E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.45965E-01  B  3.54035E-01
 Sublattice  4,  Number of sites  2.5000E-01
```

```
 A  6.45965E-01  B  3.54035E-01

 LRO#3                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 7.3238E-01, Mass 7.3238E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  5.72756E-01  B  4.27244E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.99661E-01  B  3.38612E-04
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.99661E-01  B  3.38612E-04
 Sublattice  3,  Number of sites  2.5000E-01
 B  8.54150E-01  A  1.45850E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  8.54150E-01  A  1.45850E-01
POLY:Hit RETURN to continue
POLY: 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: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    23 ITS,  CPU TIME USED   0 SECONDS
POLY: 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                    ORD    Status ENTERED   Driving force -3.9691E-02
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.68667E-01  B  3.31333E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.91453E-01  B  1.08547E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99690E-01  A  3.09926E-04

 LRO#2                    DISORD Status ENTERED   Driving force -4.9687E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.39146E-01  B  3.60854E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.39146E-01  B  3.60854E-01

 LRO#3                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  6.00000E-01  B  4.00000E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.98449E-01  B  1.55066E-03
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.98449E-01  B  1.55066E-03
 Sublattice  3,  Number of sites  2.5000E-01
 B  9.92271E-01  A  7.72920E-03
 Sublattice  4,  Number of sites  2.5000E-01
 B  6.04628E-01  A  3.95372E-01
POLY:Hit RETURN to continue
POLY: s-c x(b)=.33
   ... the command in full is SET_CONDITION
POLY: s-s-c lro *
   ... the command in full is SET_START_CONSTITUTION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    23 ITS,  CPU TIME USED   0 SECONDS
POLY: 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                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 7.8876E-02, Mass 7.8876E-01, Volume fraction 0.0000E+00  Mole fractions:
 A  6.87496E-01  B  3.12504E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.16558E-01  B  8.34422E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.16558E-01  B  8.34422E-02
 Sublattice  3,  Number of sites  2.5000E-01
```

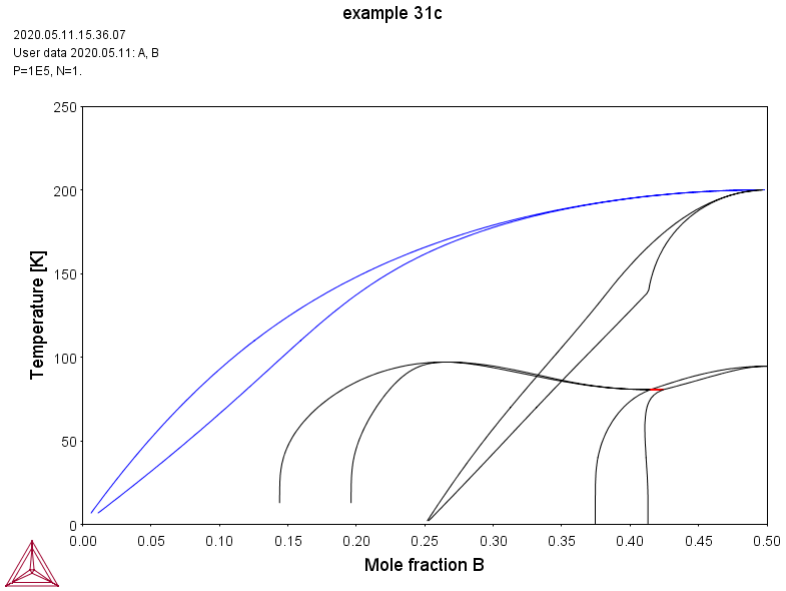
```
 A  9.16558E-01  B  8.34422E-02
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99689E-01  A  3.11152E-04

 LRO#2                   DISORD Status ENTERED   Driving force -4.8130E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.61498E-01  B  3.38502E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.61498E-01  B  3.38502E-01

 LRO#3                   ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 9.2112E-01, Mass 9.2112E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.68502E-01  B  3.31498E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.82295E-01  B  1.77045E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.82295E-01  B  1.77045E-02
 Sublattice  3,  Number of sites  2.5000E-01
 B  9.99255E-01  A  7.44800E-04
 Sublattice  4,  Number of sites  2.5000E-01
 A  7.08671E-01  B  2.91329E-01
POLY:Hit RETURN to continue
POLY: s-a-v 2 t 0 250 5
   ... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY: save tcex31c y
   ... the command in full is SAVE_WORKSPACES
POLY:
POLY: add -1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY:
POLY: 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:
POLY:
POLY:Hit RETURN to continue
POLY: 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
 MAPPING TERMINATED 1
 *** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex31\tcex31c.POLY3
 CPU time for mapping                    0 seconds
POLY: @@ Add the A2/L1_2 line
POLY: read tcex31c
   ... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:
POLY: s-c x(b)=.15 t=110
   ... the command in full is SET_CONDITION
POLY: s-a-s f
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
    38 ITS,  CPU TIME USED   0 SECONDS
POLY: 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                   ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 7.2552E-01, Mass 7.2552E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  8.40743E-01  B  1.59257E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
```

```
 A  9.74694E-01  B  2.53056E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.74694E-01  B  2.53056E-02
 Sublattice  3,  Number of sites  2.5000E-01
 A  9.74694E-01  B  2.53056E-02
 Sublattice  4,  Number of sites  2.5000E-01
 B  5.61112E-01  A  4.38888E-01

 LRO#2                    ORD    Status ENTERED   Driving force -8.9177E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.31106E-01  B  3.68894E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.99208E-01  B  7.91782E-04
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.99208E-01  B  7.91782E-04
 Sublattice  3,  Number of sites  2.5000E-01
 B  7.36997E-01  A  2.63003E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  7.36997E-01  A  2.63003E-01

 LRO#3                    DISORD Status ENTERED   Driving force  0.0000E+00
 Moles 2.7448E-01, Mass 2.7448E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  8.74469E-01  B  1.25531E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  8.74469E-01  B  1.25531E-01
 Sublattice  2,  Number of sites  2.5000E-01
 A  8.74469E-01  B  1.25531E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  8.74469E-01  B  1.25531E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  8.74469E-01  B  1.25531E-01
POLY:Hit RETURN to continue
POLY:
POLY: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY: 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
 CALCULATED    67 EQUILIBRIA

 Phase region boundary   1 at:   1.593E-01  1.100E+02
     LRO#1
  ** LRO#3
 MAPPING TERMINATED 1
 CALCULATED    57 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: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex31\tcex31c.POLY3
 CPU time for mapping                     1 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-s x n 0 .5
   ... the command in full is SET_SCALING_STATUS
POST: @@ Usually some 2nd order lines also appear
POST: set-title example 31b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
```

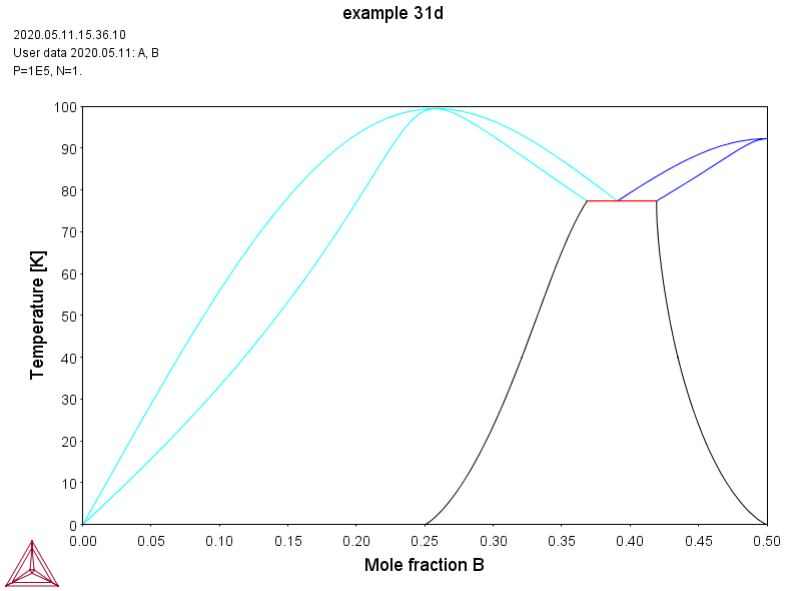
```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex31 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: set-title example 31c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



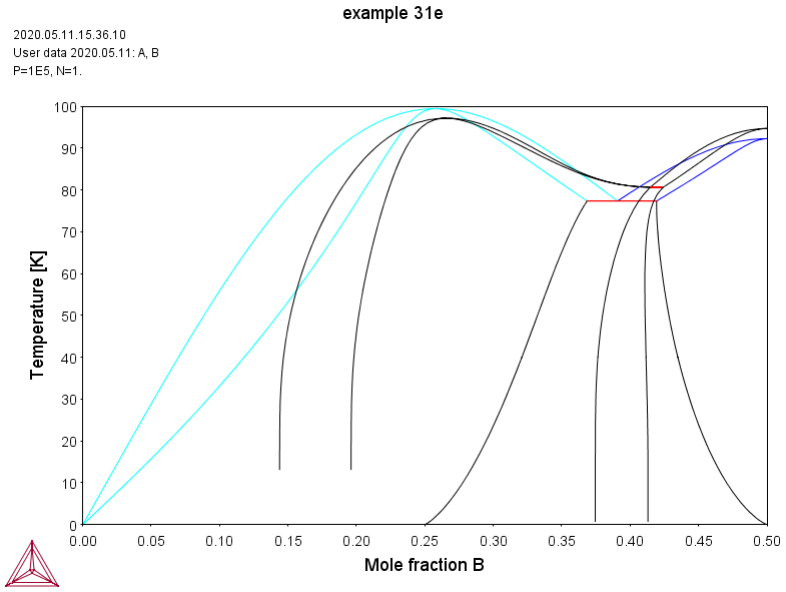

```
POST:
POST:Hit RETURN to continue
POST: ba
   ... the command in full is BACK
POLY: read tcex31c
   ... the command in full is READ_WORKSPACES
POLY: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
GES: @@ Now add a reciprocal parameter to LRO which describes
GES: @@ the SRO contribution.  The default value of this is
GES: @@ the bond energy. One can have 3 different parameters
GES: @@ depending on if one is at 25%B, 50%B or 75%B.  Here
GES: @@ we just take the 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
```

```
      G(LRO,A:A:*:*;0) = 0.0
      G(LRO,A:*:A:*;0) = 0.0
      G(LRO,A:*:*:A;0) = 0.0
      G(LRO,*:A:A:*;0) = 0.0
      G(LRO,*:A:*:A;0) = 0.0
      G(LRO,*:*:A:A;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
GES: @@ the disordered state as the contribution from the ordered
GES: @@ phase is zero there. But it is in the disordered state that
GES: @@ the SRO contribution to the Gibbs energy is most important.
GES: @@ We must add regular solution parameters to the FCC phase
GES: @@ giving the same contribution.  These can be derived by
GES: @@ setting all site-fractions for the same element equal,
GES: @@ i.e. the disordered state.
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)
& 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: c-st p lro#3=e 0
   ... the command in full is CHANGE_STATUS
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=70, P=1E5, N=1., X(B)=0.33
 DEGREES OF FREEDOM 0
POLY:
POLY: s-c t=40
   ... the command in full is SET_CONDITION
POLY: s-a-s f
   ... the command in full is SET_ALL_START_VALUES
 Forcing automatic start values
 Automatic start values will be set
POLY: 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: 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                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 9.1974E-01, Mass 9.1974E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.79151E-01  B  3.20849E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  3,  Number of sites  2.5000E-01
 A  9.05532E-01  B  9.44682E-02
 Sublattice  4,  Number of sites  2.5000E-01
 B  9.99993E-01  A  6.81574E-06

 LRO#2                   DISORD Status ENTERED   Driving force -3.8166E-01
 Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 A  6.26318E-01  B  3.73682E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01
 Sublattice  2,  Number of sites  2.5000E-01
```

```
 A  6.26318E-01  B  3.73682E-01
 Sublattice  3,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01
 Sublattice  4,  Number of sites  2.5000E-01
 A  6.26318E-01  B  3.73682E-01

 LRO#3                    ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 8.0263E-02, Mass 8.0263E-01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.65144E-01  B  4.34856E-01
 Constitution:
 Sublattice  1,  Number of sites  2.5000E-01
 A  9.99996E-01  B  4.15407E-06
 Sublattice  2,  Number of sites  2.5000E-01
 A  9.99996E-01  B  4.15407E-06
 Sublattice  3,  Number of sites  2.5000E-01
 B  8.69708E-01  A  1.30292E-01
 Sublattice  4,  Number of sites  2.5000E-01
 B  8.69708E-01  A  1.30292E-01
POLY:Hit RETURN to continue
POLY: save tcex31d y
   ... the command in full is SAVE_WORKSPACES
POLY:
POLY: list-ini-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
POLY:
POLY:
POLY:Hit RETURN to continue
POLY: 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
 *** SORRY CANNOT CONTINUE ***    4

 CALCULATED    34 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
 Terminating at diagram limit
 CALCULATED    90 EQUILIBRIA
 *** LAST BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex31\tcex31d.POLY3
 CPU time for mapping                     1 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: set-title example 31d
POST: s-s y n
   ... the command in full is SET_SCALING_STATUS
MIN VALUE : 0 100
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex31 0; 1;
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-title example 31e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex32

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex32\tcex32.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating oxide layers on steel
SYS:
SYS: @@ This example calculates oxide layers on a steel and
SYS: @@ shows how to append databases.
SYS:
SYS: @@ Note that both a TCFE and SSUB database license is
SYS: @@ required to run the example.
SYS:
SYS: set-log ex32,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw tcfe9
   ... the command in full is SWITCH_DATABASE
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: d-sys fe cr c v mn si
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
 V                       MN                      SI
   DEFINED
TDB_TCFE9: rej ph /all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                BCC_A2
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    MC_ETA
 KSI_CARBIDE             Z_PHASE                 FE4N_LP1
 FECN_CHI                SIGMA                   HIGH_SIGMA
 CHI_A12                 LAVES_PHASE_C14         M3SI
 MN9SI2                  MN11SI19                MN6SI
 G_PHASE                 CR3SI                   FE2SI
 FESI2_H                 FESI2_L                 MSI
 M5SI3                   CO3VV                   NB5SI3_D8L
 MSI2_C40                M11SI8                  M6SI5
 AL4C3                   FE8SI2C                 SIC
 MN5SIC                  CRZN17                  CUZN_EPSILON
 AL5FE4                  MP_B31                  M2P_C22
 FLUORITE_C1:I           ZRO2_TETR:I             M2O3C:I
 M2O3H:I   REJECTED
TDB_TCFE9: rest ph fcc_a1 bcc_a2 hcp_a3 m23 m7 cementite
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  HCP_A3
 M23C6                   M7C3                    CEMENTITE
   RESTORED
TDB_TCFE9: get
   ... the command in full is GET_DATA
15:37:30,282 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set HCP_A3#2
   ... 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, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'C. Qiu, ISIJ International, 32 (1992) 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  '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'
  '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'
  'B. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-C'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
```

```
      1989); C-FE-MN'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223;
      Fe-Si and Fe-Si-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
  'Thermo-Calc Software, Sweden, 2019: Volume data updated for TCFE9
      database (TCFE v9.1, June, 2019).'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
  'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6
      database (TCFE v6, April, 2008).'
  'W. Huang, TRITA-MAC 431 (1990); C-V'
  'A. Fernandez Guillermet and W. Huang, TRITA-MAC 440 (1990); Mn-V-C'
  'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53,
      105-125; Molar volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
  'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'B.-J. Lee, TRITA-MAC 474 (1991); Cr-Fe-V'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
  'W. Huang, TRITA-MAC 432 (Rev 1989,1990); FE-V'
  'J-O. Andersson, CALPHAD, 7 (1983) 305-315 (Parameters revised 1986 due to
      new decription of V) TRITA 0201 (1982); FE-V'
  'W. Huang, TRITA-MAC 432 (1990); C-Fe-V'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'W. Huang, TRITA-MAC 439 (1990) also in W. Huang, CALPHAD, 15, 195
      -208(1991); Mn-V, Fe-Mn-V'
  'W. Huang, TRITA-MAC 441 (1990) also in W. Huang, Metall. Trans. A, 22A,
      1911-20(1991); Fe-Mn-V-C'
  'M.H. Rand and N. Saunders, COST 507 Report (1998); Si-V'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'B.-J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
      M23C6'
  'B.-J. Lee, TRITA-MAC 475 (1991); C-Cr-Fe-V'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-V-C'
  'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe
      -Si-C'
  'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; C-Cr-Fe-V'
 -OK-
TDB_TCFE9: @@ All oxides from the substance database
TDB_TCFE9: app ssub5
   ... the command in full is APPEND_DATABASE
 Current database: SGTE Substances Database v5.2

 VA  DEFINED
APP:
APP: d-sys fe cr v si mn o c
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      V
 SI                      MN                      O
 C  DEFINED
APP: get
   ... the command in full is GET_DATA
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

   C1<G> T.C.R.A.S. Class: 1
      C1<G> C<G>
   C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      C1O1<G> CO<G>
      CARBON MONOXIDE <GAS>
      STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
   C1O2<G> T.C.R.A.S. Class: 2
      C1O2<G> CO2<G>
      CARBON DIOXIDE <GAS>
   C1SI1<G> T.C.R.A.S. Class: 5
      C1SI1<G> SiC<G>
      SILICON CARBIDE <GAS>
   C1SI2<G> T.C.R.A.S. Class: 6
      C1SI2<G> Si2C<G>
      DISILICON CARBIDE <GAS>
   C1SI3<G> THERMODATA 02/94 BC
      C1SI3<G> Si3C<G>
   C1SI4<G> THERMODATA 02/94 BC
      C1SI4<G> Si4C<G>
   C2<G> T.C.R.A.S. Class: 2
      C2<G>
      CARBON Diatomic Gas.
   C2O1<G> T.C.R.A.S. Class: 5
      C2O1<G> C2O<G>
   C2SI1<G> JANAF THERMOCHEMICAL TABLES SGTE **
      C2SI1<G> SiC2<G>
      PUBLISHED BY JANAF AT 3/67
   C2SI2<G> THERMODATA 02/94 BC
      C2SI2<G> Si2C2<G>
   C2SI3<G> THERMODATA 03/94 BC
      C2SI3<G> Si3C2<G>
   C3<G> T.C.R.A.S. Class: 6
      C3<G>
      CARBON <TRIATOMIC GAS>
   C3O2<G> T.C.R.A.S. Class: 6
      C3O2<G>
   C4<G> T.C.R.A.S. Class: 7
```

C4<G>
C5<G> T.C.R.A.S. Class: 7
C5<G>
C5FE1O5<G> JANAF 1982 SGTE
C5FE1O5<G> Fe(CO)5<G>
IRON PENTACARBONYL <GAS>
ASSESSMENT DATED 3/78
C60<G> MHR-95
C60<G>
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the rotational
data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that
a frequency with degeneracy 5 is missing from list in [94Kor/Sid];
taken to be 419 cm-1, which gives very good, though not exact,
agreement with values quoted in [94Kor/Sid]. Note discrepancy
between calculated DrS(298) = -8943.5 J mol K-1 for the reaction
60C<g>=C60<g>and that given by [94Kor/Sid] in their Table 5,
-8950 J mol K-1. Enthalpy of formation: DfH = 2588 kJ/mol from
DsubH(298.15K) = 166 +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure
values reproduced very well.
[91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).
CR1<G> THERMODATA
CR1<G> Cr<G>
New Assessment (H_form and S only)
CR1O1<G> T.C.R.A.S. Class: 5
CR1O1<G> CrO<G>
CR1O2<G> T.C.R.A.S. Class: 6
CR1O2<G> CrO2<G>
CHROMIUM DIOXIDE <GAS>
CR1O3<G> T.C.R.A.S. Class: 6
CR1O3<G> CrO3<G>
CHROMIUM TRIOXIDE <GAS>
CR2<G> THERMODATA
CR2<G> Cr2<G>
New assessment (H_form and S only)
CR2O1<G> T.C.R.A.S. Class: 6
CR2O1<G> Cr2O<G>
CR2O2<G> T.C.R.A.S. Class: 6
CR2O2<G> Cr2O2<G>
CR2O3<G> T.C.R.A.S. Class: 7
CR2O3<G> Cr2O3<G>
CHROMIUM<3> OXIDE <GAS>
FE1<G> THERMODATA
FE1<G> Fe<G>
Data provided by T.C.R.A.S. October 1996
Modified by Thermodata - new assessment
FE1O1<G> TCRAS 5-F FEO IRON OXIDE 23/11/06
FE1O1<G> FeO<G>
FE1O2<G> T.C.R.A.S Class: 6
FE1O2<G> FeO2<G>
Data provided by TCRAS. October 1996. Error in version 1997.
S298 corrected to 1bar
20080222 AAZ TCRAS2006 : dH, S
FE2<G> THERMODATA
FE2<G> Fe2<G>
Data provided by T.C.R.A.S. October 1996
Modified by Thermodata - new assessment.
Typing error corrected 12/06
MN1<G> THERMODATA 01/93
MN1<G> Mn<G>
MANGANESE <GAS>
28/01/93
MN1O1<G> T.C.R.A.S. Class: 2
MN1O1<G> MnO<G>
MANGANESE<2> OXIDE <GAS>
MN1O2<G> T.C.R.A.S. Class: 7
MN1O2<G> MnO2<G>
MANGANESE<4> OXIDE <GAS>
O1<G> TCRAS 02/06/80
O1<G> O<G>
O10V4<G> T.C.R.A.S. Class: 7
O10V4<G> V4O10<G>
O1SI1<G> T.C.R.A.S. Class: 1
O1SI1<G> SiO<G>
SILICON <MONOXIDE GAS>
O1V1<G> T.C.R.A.S. Class: 5
O1V1<G> VO<G>
VANADIUM MONOXIDE <GAS>
O2<G> TCRAS 21/06/90
O2<G>
OXYGEN Gaseous Standard State.
O2SI1<G> T.C.R.A.S. Class: 5
O2SI1<G> SiO2<G>
SILICON DIOXIDE <GAS>
O2SI2<G> CHATILLON(1995)
O2SI2<G> Si2O2<G>
Hf from mass spectrometry Zmbov K.F., Ames L.L., Margrave J.L., High
Temp. Sci. 5 (1973)235 and Rocabois Ph., Chatillon C. , Bernard. C.
Rev. Int. Hautes Temper. Refract. Fr. 28 (1992-93) 37-48 and Cp, S(T)
an
Fef from Al2O2<G> according to Al2O2 by Dimensional Model (Frurip and Bl
O2V1<G> T.C.R.A.S. Class: 5
O2V1<G> VO2<G>
VANADIUM DIOXIDE <GAS>
O3<G> TCRAS 02/06/80
O3<G>
OZONE Gaseous Standard State.
SI1<G> T.C.R.A.S. Class: 1
SI1<G> Si<G>
SILICON <GAS>
SI2<G> T.C.R.A.S. Class: 5
SI2<G> Si2<G>
SILICON <DIATOMIC GAS>
SI3<G> T.C.R.A.S. Class: 6
SI3<G> Si3<G>
SILICON <TRIATOMIC GAS>
V1<G> T.C.R.A.S. Class: 1
V1<G> V<G>
VANADIUM <GAS>
O2SI1<BETA-QUARTZ> N.P.L.
O2SI1_BETA_QUARTZ SiO2_BETA_QUARTZ
Data from an assessment by T I Barry, reported in paper on CaO-SiO2
system by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
C0.88V1 THERMODATA 01/93
C0.88V1 VC0.88
28/01/93

C1FE1O3 N.P.L. SGTE **
C1FE1O3 FeCO3 Siderite
IRON<2> CARBONATE
DECOMPOSES BEFORE FUSION.
C1FE3 N.P.L. SGTE **
C1FE3 Fe3C Cementite
CEMENTITE
C1MN1O3 KUBASCHEWSKI EVANS ALCOCK 1967 SGTE **
C1MN1O3 MnCO3
MANGANESE<2> CARBONATE
C1MN3 M. ANCEY, Y. DENIEL SGTE
C1MN3 Mn3C
TRIMANGANESE MONOCARBIDE
C1SI1<C1SI1_ALPHA> JANAF THERMOCHEMICAL TABLES SGTE **
C1SI1_ALPHA SiC_ALPHA
N CARBIDE <ALPHA>
ALPHA-SIC . HEX.FORM . PUBL. BY JANAF AT 3/67 .LESS STABLE THAN
SIC_BETA UP TO 2200K. Decomposes to complex vapour at about 3259K.
C1SI1<C1SI1_BETA> JANAF THERMOCHEMICAL TABLES SGTE
C1SI1_BETA SiC_BETA
N CARBIDE <BETA>
CUBIC FORM OF TYPE ZNS. STABLE WITH RESPECT TO SIC-ALPHA UP TO 2200K.
PUBL. BY JANAF 03/67
C1V2 THERMODATA 01/93
C1V2 V2C
DIVANADIUM MONOCARBIDE
28/01/93 Tm=2438 K.
C2CR3 JANAF THERMOCHEMICAL TABLES SGTE
C2CR3 Cr3C2
3-CHROMIUM 2-CARBIDE
(1975 SUPPL.) PUBLISHED BY JANAF AT 12/73
Melts incongruently at 2168K.
C2MN5 T.C.R.A.S. Class: 7
C2MN5 Mn5C2
C3CR7 JANAF THERMOCHEMICAL TABLES SGTE **
C3CR7 Cr7C3
7-CHROMIUM 3-CARBIDE
PUBLISHED BY JANAF AT 12/73 .REVISED VALUE FOR DELTA H 298
BY B.UHRENIUS 1980 Melts incongruently at 2053K.
C3MN7 S.G.T.E. SGTE **
C3MN7 Mn7C3
HEPTAMANGANESE TRICARBIDE
REASSESMENT BY B.URHENIUS
C5FE1O5<L> I. BARIN 3rd. Edition
C5FE1O5_Liquid Fe(CO)5_Liquid
IRON PENTACARBONYL (Liquid). Same as in previous versions.
Rounding of H298.
C60 MHR-95
C60
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.
The
Fitted to the data in [94Kor/Sid], who took the phase transition at
257K
that [94Kor/Sid] do not give an explicit value for S(298.15K).
S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =425.8 and Cp
e
calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]
in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.
Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
the value preferred, if obliquely, by [94Kor/Sid].
[92Ste/Chi]W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,
P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).
C6CR1O6 I. BARIN 3rd. Edition
C6CR1O6 Cr(CO)6
CHROMIUM HEXACARBONYL
SUBLIMATION AT 424K.
C6CR23 JANAF THERMOCHEMICAL TABLES SGTE
C6CR23 Cr23C6
23-CHROMIUM 6-CARBIDE
((1975 SUPPL.)) PUBLISHED BY JANAF AT 12/73
Melts incongruently at 1793K.
C6MN23 T.C.R.A.S. Class: 7
C6MN23 Mn23C6
CR1O2 S.G.T.E. SGTE **
CR1O2 CrO2
CHROMIUM DIOXIDE
O.KUBASCHEWSKI'S REASSESSMENT 1979
CR1O3 S.G.T.E. SGTE **
CR1O3 CrO3
CHROMIUM TRIOXIDE
O.KUBASCHEWSKI'S REASSESSMENT 1979
CR1SI1 T.C.R.A.S. Class: 6
CR1SI1 CrSi
CHROMIUM SILICON
CR1SI2 T.C.R.A.S. Class: 7
CR1SI2 CrSi2
CHROMIUM 2-SILICON
CR2FE1O4 KUBASCHEWSKI EVANS ALCOCK 1967 SGTE
CR2FE1O4 FeCr2O4 FeO-Cr2O3
DELTAH 298 CALCULATED FROM OXIDES =-13100CAL/MOL(#1000)
CR2O3 T.C.R.A.S. Class: 7
CR2O3 Cr2O3
CHROMIUM<3> OXIDE
cp refitted by AP because of low T FC at 306K
CR3SI1 T.C.R.A.S. Class: 7
CR3SI1 Cr3Si
3-CHROMIUM 2-SILICON
CR5O12 S.G.T.E. SGTE **
CR5O12 Cr5O12
5-CHROMIUM 12-OXIDE
CR5O12: 5-CHROMIUM 12-OXIDE **DECOMPOSITION (643 -->705 K)
O.KUBASCHEWSKI'S REASSESSMENT 1979.
CR5SI3 T.C.R.A.S. Class: 7
CR5SI3 Cr5Si3
5-CHROMIUM 3-SILICON
CR8O21 S.G.T.E. SGTE **
CR8O21 Cr8O21
8-CHROMIUM 21-OXIDE
O.KUBASCHEWSKI'S REASSESSMENT 1971
CR8O21 8-CHROMIUM 21-OXIDE,DECOMPOSITION (600 --> 640K.)
O2SI1<CRISTOBALITE> N.P.L.
O2SI1_CRISTOBALITE SiO2_CRISTOBALITE
Data from an assessment by T I Barry, reported in paper on CaO-SiO2
syst
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
CR1 S.G.T.E. **

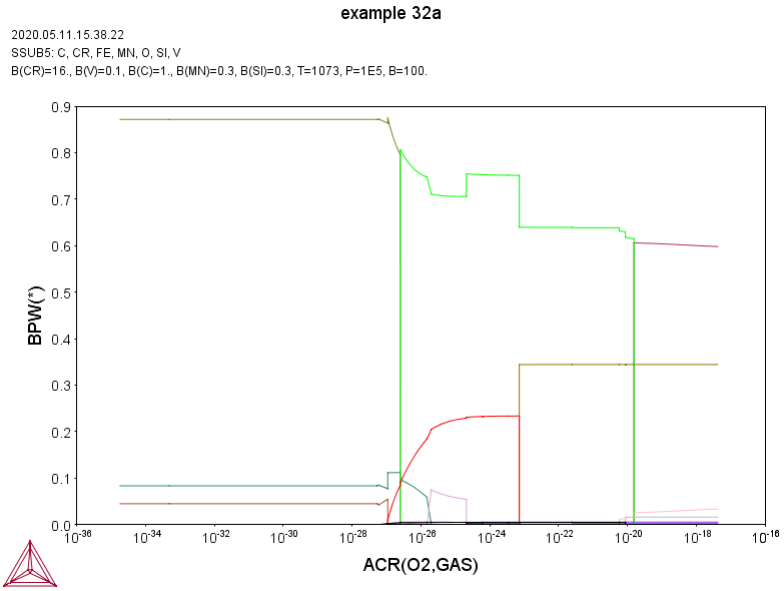
CR1 Cr
Data from SGTE Unary DB
C1<DIAMOND> S.G.T.E. **
C_DIAMOND
<DIAMOND>
Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken
from 1994 database (ex THERMODATA 01/93)
FE2O4SI1<FAYALITE> S.G.T.E.
FE2O4SI1 Fe2SiO4 FAYALITE 2FeO-SiO2
IRON ORTHOSILICATE <FAYALITE>
Data assessed by M. Selleby. 20/5/94
FE1O1 T.C.R.A.S Class: 5
FE1O1 FeO FeO_Wustite
IRON OXIDE. Data provided by T.C.R.A.S. in 2000
FE1O3SI1 THERMODATA 01/93
FE1O3SI1 FeSiO3 FeO-SiO2
28/01/93
FE1O4V2 THERMODATA 01/93
FE1O4V2 FeV2O4 FeO-V2O3
28/01/93
FE1O6V2 THERMODATA 01/93
FE1O6V2 FeV2O6 FeO-V2O5
IRON VANADATE
28/01/93 Td = 1023 K.
FE1SI1 THERMODATA 01/93
FE1SI1 FeSi
IRON SILICIDE
28/01/93
FE1SI2.33 THERMODATA 01/93
FE1SI2.33 FeSi2.33
LEBOITE <ALPHA>
28/01/93 LEBOITE (ALPHA).
FE1SI2 THERMODATA 01/93
FE1SI2 FeSi2
LEBOITE <BETA>
28/01/93 LEBOITE (BETA). Td = 1243K
FE2MN1O4 O. KUBASCHEWSKI DCS REPORT 7 . SGTE
FE2MN1O4 MnFe2O4 MnO-Fe2O3
MANGANESE DIIRON TETRAOXIDE
BARIN
KNACKE ED 73 REF *,5,1 (KUBASCHEWSKI) .
FE2O3<FE2O3_GAMMA> T.C.R.A.S Class: 5
FE2O3_GAMMA Fe2O3_Gamma
Data provided by T.C.R.A.S. in 2000
FE1 S.G.T.E. **
FE1 Fe
Data from SGTE Unary DB
C1<GRAPHITE> S.G.T.E. **
C_GRAPHITE
Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95
FE2O3<HEMATITE> T.C.R.A.S Class: 7
FE2O3 Fe2O3 Hematite
Data provided by T.C.R.A.S. in 2000 with previous description
of the magnetic transition fitted by IA. In version 2000 only
H298 has been changed.
FE3O4<MAGNETITE> JANAF 4th Ed.
FE3O4 Fe3O4 MAGNETITE
Data refitted by IA to reproduce the magnetic transition.
MN11SI19 N.P.L. FEB. 1994
MN11SI19 Mn11Si19
MN1O1 I. BARIN 3rd. Edition
MN1O1 MnO
MANGANESE OXIDE.Data taken from BARIN 3rd. Ed. (1995)
MN1O2 I. BARIN 3rd. Edition
MN1O2 MnO2
MANGANESE<4> OXIDE. Data taken from BARIN 3rd. Ed. (1995).
S(298) FROM N.P.L.
MN1SI1 T.G. CHART NPL REPORT.CHEM.18 AUGUST 197 SGTE
MN1SI1 MnSi
MANGANESE SILICON
S(298.15) CALCULATED FROM CHART'S PUBLISHED VALUE FOR DELTA S(298.15)
FORMATION AND HULTGREN'S DATA OF S(298.15) FOR SI AND CR (REF.4)
MN2O3 KUBASCHEWSKI EVANS ALCOCK 1967 SGTE **
MN2O3 Mn2O3
MANGANESE<3> OXIDE
DATA CORRESPONDS TO MNO1.5-1.6. DECOMPOSITION BEFORE MELTING.
MN2O7<L> T.C.R.A.S. Class: 7
MN2O7 Mn2O7
MN3O4 KUBASCHEWSKI DCS REPORT 7 . SGTE
MN3O4 Mn3O4 MnO-Mn2O3
MANGANESE<2,3> OXIDE
MNO(1.33-1.41) .
MN3SI1 N.P.L. FEB. 1994
MN3SI1 Mn3Si
3-MANGANESE SILICON
MN4SI7 T.G. CHART NPL REPORT.CHEM.18 AUG 1997 SGTE
MN4SI7 Mn4Si7
S(298.15) CALCULATED FROM CHART'S PUBLISHED VALUE FOR DELTA S(298.15)
FORMATION AND HULTGREN'S DATA OF S(298.15) FOR SI AND CR (REF.4)
MN5SI3 T.G. CHART NPL REPORT.CHEM.18 AUG 1997 SGTE
MN5SI3 Mn5Si3
5-MANGANESE 3-SILICON
S(298.15) CALCULATED FROM CHART'S PUBLISHED VALUE FOR DELTA S(298.15)
FORMATION AND HULTGREN'S DATA OF S(298.15) FOR SI AND CR (REF.4)
MN1 S.G.T.E. **
MN1 Mn
Data from SGTE Unary DB
O1V1 T.C.R.A.S. Class: 6
O1V1 VO
VANADIUM MONOXIDE
O3V2 T.C.R.A.S. Class: 6
O3V2 V2O3
VANADIUM TRIOXIDE
O4V2 T.C.R.A.S. Class: 7
O4V2 V2O4<G> (VO2)2<G>
O5V2 T.C.R.A.S. Class: 7
O5V2 V2O5
VANADIUM PENTOXIDE
O2SI1<QUARTZ> N.P.L.
O2SI1_QUARTZ SiO2_Quartz SiO2_Alpha_Quartz
Data from an assessment by T I Barry, reported in paper on CaO-SiO2
syst
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
MN1O3SI1<RHODONITE> I. BARIN 3rd. Edition
MN1O3SI1 MnSiO3 RHODONITE MnO-SiO2
MANGANESE METASILICATE <RHODONITE> .Data taken from BARIN 3rd.

```
      Ed. (1995)
   SI1V3 THERMODATA 10/85 BC
      SI1V3 SiV3
   SI2V1 T.G. CHART NPL REPORT.CHEM.18 AUGUST 197 SGT
      SI2V1 VSi2
      VANADIUM 2-SILICON
      S(298.15) CALCULATED FROM CHART'S PUBLISHED VALUE FOR DELTA S(298.15)
      FORMATION AND HULTGREN'S DATA OF S(298.15) FOR SI AND CR (REF.4)
   SI3V5 THERMODATA 10/85
      SI3V5 V5Si3
   O2SI1<SIO2_LIQUID> N.P.L.
      O2SI1_LIQUID SiO2_Liquid
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   SI1 JANAF THERMOCHEMICAL TABLES SGTE **
      SI1 Si
      SILICON
      PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
      --U.D. 31/10/85
   MN2O4SI1<TEPHROITE> I. BARIN 3rd. Edition
      MN2O4SI1 Mn2SiO4 TEPHROITE 2MnO-SiO2
      MANGANESE ORTHOSILICATE <TEPHROITE>. H298, S298 and Tmax modified
   O2SI1<TRIDYMITE> N.P.L.
      O2SI1_TRIDYMITE SiO2_TRIDYMITE
      Data from an assessment by T I Barry, reported in paper on CaO-SiO2
      syst
      by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88
   V1 S.G.T.E. **
      V1 V
      VANADIUM
      Data from SGTE Unary DB
   FE0.947O1<WUSTITE> T.C.R.A.S Class: 5
      FE0.947O1 Fe0.947O WUSTITE
      WUSTITE. Data provided by T.C.R.A.S. in 2000
      20080222 AAZ TCRAS2006 : dH, S
 -OK-
15:37:42,465 WARN  Different masses detected in databases: Si
APP: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:

POLY: 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: 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:
POLY: @@set-start-value y(fcc_a1#2,si)=1e-2
POLY: @@set-start-value y(fcc_a1#1,si)=1e-12
POLY: set-start-const fcc#1
   ... the command in full is SET_START_CONSTITUTION
Y(FCC_A1#1,CR) /1/: 1e-6
Y(FCC_A1#1,FE) /1/: 0.999
Y(FCC_A1#1,MN) /1/: 4e-6
Y(FCC_A1#1,SI) /1/: 1e-9
Y(FCC_A1#1,V) /1/: 5e-7
Y(FCC_A1#1,C#2) /1/: 4e-2
Y(FCC_A1#1,VA#2) /1/: 0.96
POLY: set-start-const fcc#2
   ... the command in full is SET_START_CONSTITUTION
Y(FCC_A1#2,CR) /1/: 2e-2
Y(FCC_A1#2,FE) /1/: 0.4
Y(FCC_A1#2,MN) /1/: 7e-4
Y(FCC_A1#2,SI) /1/: 4e-4
Y(FCC_A1#2,V) /1/: 0.6
Y(FCC_A1#2,C#2) /1/: 0.8
Y(FCC_A1#2,VA#2) /1/: 0.2
POLY:Hit RETURN to continue
POLY: @@ We have atomic oxygen as a component. Later we use the
POLY: @@ partial pressure of O2 as output. The state variable
POLY: @@ LNACR is the chemical potential divided by RT, usual
POLY: @@ values are between -40 and 0
POLY:
POLY: s-c lnacr(o)=-27
   ... the command in full is SET_CONDITION
POLY: s-r-s o gas * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated         10692 grid points in             1 s
   131 ITS,  CPU TIME USED  12 SECONDS
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: SSUB5

 Conditions:
 B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100,
    LNACR(O)=-27
 DEGREES OF FREEDOM 0

 Temperature   1073.00 K (   799.85 C),  Pressure  1.000000E+05
 Number of moles of components  2.23271E+00,  Mass in grams  1.00000E+02
 Total Gibbs energy -2.78609E+05,  Enthalpy -1.28397E+05,  Volume  9.84580E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       8.3257E-02  1.0000E-02 1.9687E-01 -1.4499E+04 SER
 CR                      3.0772E-01  1.6000E-01 5.3299E-06 -1.0833E+05 SER
 FE                      1.3332E+00  7.4453E-01 4.8258E-03 -4.7585E+04 SER
 MN                      5.4607E-03  3.0000E-03 1.0592E-07 -1.4328E+05 SER
 O                       4.9047E-01  7.8470E-02 1.8795E-12 -2.4088E+05 GAS
 SI                      1.0681E-02  3.0000E-03 7.4765E-14 -2.6965E+05 SER
 V                       1.9631E-03  1.0000E-03 2.9371E-08 -1.5473E+05 SER

 FCC_A1#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.3877E+00, Mass 7.5133E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  9.90949E-01  CR  2.94225E-04  V   6.34363E-05  O   0.00000E+00
```

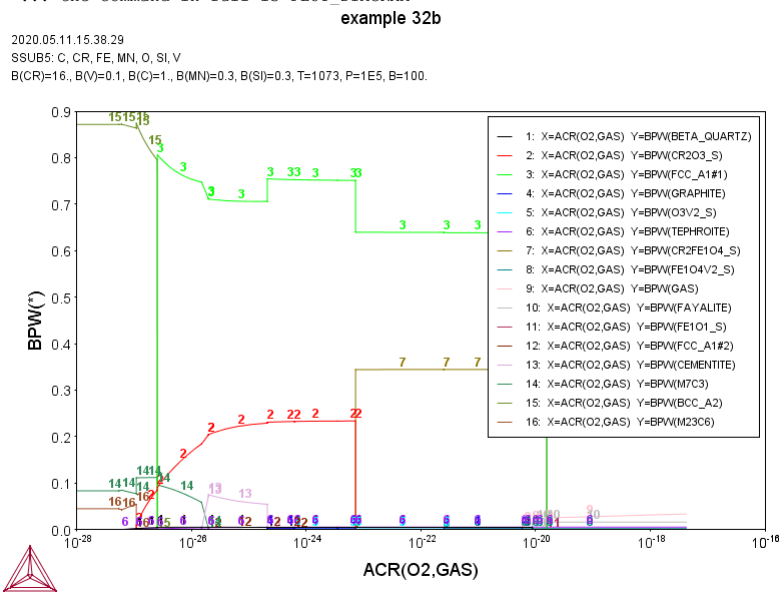
```
 C   8.62235E-03  MN  7.10657E-05  SI  1.76833E-07

 CR2O3_S                     Status ENTERED     Driving force  0.0000E+00
 Moles 7.6823E-01, Mass 2.3352E+01, Volume fraction 0.0000E+00  Mass fractions:
 CR  6.84207E-01  C   0.00000E+00  MN  0.00000E+00  V   0.00000E+00
 O   3.15793E-01  SI  0.00000E+00  FE  0.00000E+00

 TEPHROITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.8772E-02, Mass 5.4160E-01, Volume fraction 0.0000E+00  Mass fractions:
 MN  5.44054E-01  SI  1.39069E-01  V   0.00000E+00  CR  0.00000E+00
 O   3.16878E-01  C   0.00000E+00  FE  0.00000E+00

 BETA_QUARTZ                 Status ENTERED     Driving force  0.0000E+00
 Moles 2.3998E-02, Mass 4.8063E-01, Volume fraction 0.0000E+00  Mass fractions:
 O   5.32554E-01  C   0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
 SI  4.67446E-01  V   0.00000E+00  FE  0.00000E+00

 GRAPHITE                    Status ENTERED     Driving force  0.0000E+00
 Moles 2.9321E-02, Mass 3.5218E-01, Volume fraction 0.0000E+00  Mass fractions:
 C   1.00000E+00  SI  0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
 V   0.00000E+00  O   0.00000E+00  FE  0.00000E+00

 O3V2_S                      Status ENTERED     Driving force  0.0000E+00
 Moles 4.6737E-03, Mass 1.4010E-01, Volume fraction 0.0000E+00  Mass fractions:
 V   6.79762E-01  C   0.00000E+00  MN  0.00000E+00  CR  0.00000E+00
 O   3.20238E-01  SI  0.00000E+00  FE  0.00000E+00
POLY: sh lnacr(o)
   ... the command in full is SHOW_VALUE
 LNACR(O)=-27
POLY: @@ List the activity of O2
POLY: show lnacr(o2,gas)
   ... the command in full is SHOW_VALUE
 LNACR(O2,GAS)=-54
POLY:Hit RETURN to continue
POLY: @@ Vary the normalized chemical potential of oxygen
POLY: @@ between -20 and -40
POLY: 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: save tcex32 y
   ... the command in full is SAVE_WORKSPACES
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
 No initial equilibrium, using default
 Step will start from axis value   -27.0000
...OK

 Phase Region from   -27.0000     for:
     BETA_QUARTZ
     CR2O3_S
     FCC_A1#1
     GRAPHITE
     O3V2_S
     TEPHROITE
 Global check of adding phase at -2.66392E+01
 Calculated     4 equilibria

 Phase Region from   -26.6392     for:
     BETA_QUARTZ
     CR2FE1O4_S
     CR2O3_S
     FCC_A1#1
     GRAPHITE
     O3V2_S
     TEPHROITE
 Calculated     2 equilibria

 Phase Region from   -26.6392     for:
     BETA_QUARTZ
     CR2FE1O4_S
     FCC_A1#1
     GRAPHITE
     O3V2_S
     TEPHROITE
 Global check of adding phase at -2.48680E+01
 Calculated    10 equilibria

 Phase Region from   -24.8680     for:
     BETA_QUARTZ
     CR2FE1O4_S
     FCC_A1#1
     FE1O4V2_S
     GRAPHITE
     O3V2_S
     TEPHROITE
 Calculated     2 equilibria

 Phase Region from   -24.8680     for:
     BETA_QUARTZ
     CR2FE1O4_S
     FCC_A1#1
     FE1O4V2_S
     GRAPHITE
     TEPHROITE
 Global check of adding phase at -2.32956E+01
 Calculated     9 equilibria

 Phase Region from   -23.2956     for:
     GAS
     BETA_QUARTZ
     CR2FE1O4_S
     FCC_A1#1
     FE1O4V2_S
     GRAPHITE
     TEPHROITE
 Calculated     2 equilibria

 Phase Region from   -23.2956     for:
     GAS
     BETA_QUARTZ
     CR2FE1O4_S
     FCC_A1#1
```

```
    FE1O4V2_S
    TEPHROITE
Global check of adding phase at -2.30914E+01
Calculated     4 equilibria

Phase Region from   -23.0914     for:
    GAS
    BETA_QUARTZ
    CR2FE1O4_S
    FAYALITE
    FCC_A1#1
    FE1O4V2_S
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -23.0914     for:
    GAS
    CR2FE1O4_S
    FAYALITE
    FCC_A1#1
    FE1O4V2_S
    TEPHROITE
Global check of adding phase at -2.28036E+01
Calculated     4 equilibria

Phase Region from   -22.8036     for:
    GAS
    CR2FE1O4_S
    FAYALITE
    FCC_A1#1
    FE1O1_S
    FE1O4V2_S
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -22.8036     for:
    GAS
    CR2FE1O4_S
    FAYALITE
    FE1O1_S
    FE1O4V2_S
    TEPHROITE
Global test at -2.10000E+01 .... OK
Terminating at   -20.0000
Calculated    15 equilibria

Phase Region from   -27.0000     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1#1
    GRAPHITE
    O3V2_S
    TEPHROITE
Global check of adding phase at -2.78699E+01
Calculated     6 equilibria

Phase Region from   -27.8699     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1#1
    FCC_A1#2
    GRAPHITE
    O3V2_S
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -27.8699     for:
    BETA_QUARTZ
    CR2O3_S
    FCC_A1#1
    FCC_A1#2
    GRAPHITE
    TEPHROITE
Global check of adding phase at -2.84104E+01
Calculated     5 equilibria

Phase Region from   -28.4104     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1#1
    FCC_A1#2
    GRAPHITE
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -28.4104     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1#1
    FCC_A1#2
    TEPHROITE
Global check of adding phase at -2.95944E+01
Calculated     8 equilibria

Phase Region from   -29.5944     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1#1
    FCC_A1#2
    M7C3
    TEPHROITE
Calculated     2 equilibria

Phase Region from   -29.5944     for:
    BETA_QUARTZ
    CEMENTITE
    CR2O3_S
    FCC_A1#1
    M7C3
    TEPHROITE
Global check of removing phase at -2.97311E+01
Calculated     3 equilibria
```

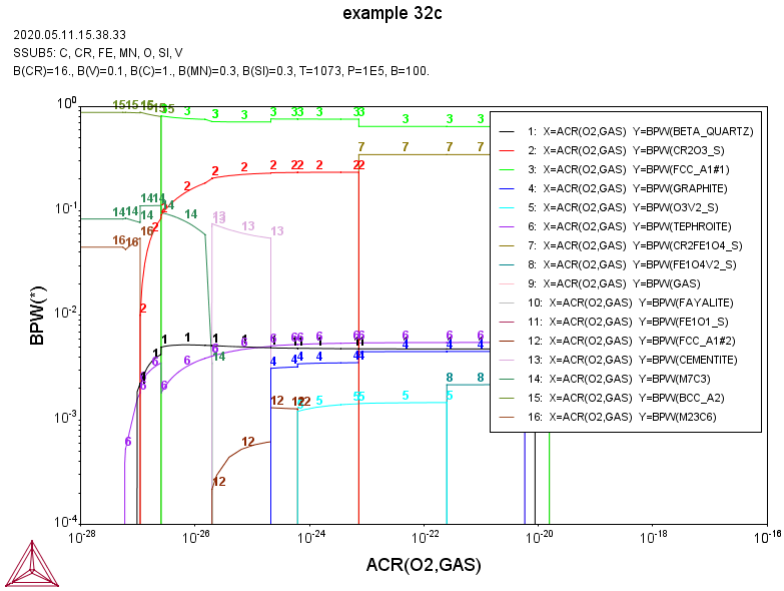
```
 Phase Region from   -29.7311     for:
     BETA_QUARTZ
     CR2O3_S
     FCC_A1#1
     M7C3
     TEPHROITE
 Global test at -3.01000E+01 .... OK
 Global test at -3.06000E+01 .... OK
 Global check of adding phase at -3.06165E+01
 Calculated    21 equilibria

 Phase Region from   -30.6165     for:
     BCC_A2
     BETA_QUARTZ
     CR2O3_S
     FCC_A1#1
     M7C3
     TEPHROITE
 Global check of removing phase at -3.06226E+01
 Calculated     3 equilibria

 Phase Region from   -30.6226     for:
     BCC_A2
     BETA_QUARTZ
     CR2O3_S
     M7C3
     TEPHROITE
 Global check of adding phase at -3.10401E+01
 Calculated    10 equilibria

 Phase Region from   -31.0401     for:
     BCC_A2
     BETA_QUARTZ
     CR2O3_S
     M23C6
     M7C3
     TEPHROITE
 Global check of removing phase at -3.10401E+01
 Calculated     3 equilibria

 Phase Region from   -31.0401     for:
     BCC_A2
     BETA_QUARTZ
     M23C6
     M7C3
     TEPHROITE
 Global check of removing phase at -3.13345E+01
 Calculated     4 equilibria

 Phase Region from   -31.3345     for:
     BCC_A2
     M23C6
     M7C3
     TEPHROITE
 Global check of removing phase at -3.13894E+01
 Calculated     4 equilibria

 Phase Region from   -31.3894     for:
     BCC_A2
     M23C6
     M7C3
 Global test at -3.33500E+01 .... OK
 Global test at -3.58500E+01 .... OK
 Global test at -3.83500E+01 .... OK
 *** Buffer saved on file:
 c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex32\tcex3
 2.POLY3
 Terminating at   -40.0000
 Calculated    38 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex32\tcex32.POLY3
POLY:
POLY: po
   ... the command in full is POST
  POLY-3 POSTPROCESSOR VERSION 3.2
POST:
POST: s-d-a x acr(o2,gas)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y bpw(*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-a-ty
   ... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : x
AXIS TYPE /LINEAR/: log
POST: set-title example 32a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



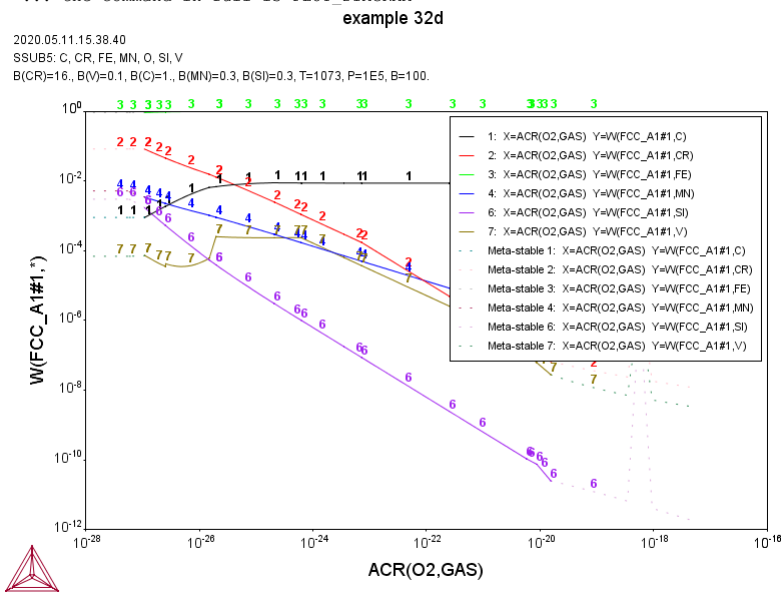

```
POST:
POST:Hit RETURN to continue
POST: s-lab f
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-s x n 1e-28 1e-18
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 32b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y
   ... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: s-s y n 1e-4 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 32c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ Finally plot how the composition of FCC varies.
POST: s-d-a y w(fcc_a1#1,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-s y n 1e-12 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 32d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex33

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex33\tcex33.TCM.test"
SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Benchmark calculation for Fe-Cr-C isopleth
SYS: @@
SYS: set-log ex33,,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw FEDEMO
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database v3.0

 VA                      /-  DEFINED
TDB_FEDEMO: d-sys fe cr c
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      C
   DEFINED
TDB_FEDEMO: rej ph /all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                BCC_A2
 LAVES_PHASE_C14         CBCC_A12                CEMENTITE
 CHI_A12                 CUB_A13                 DIAMOND_FCC_A4
 FCC_A1                  GRAPHITE                HCP_A3
 KSI_CARBIDE             M23C6                   M3C2
 M5C2                    M7C3                    SIGMA
   REJECTED
TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 graphite sigma cementite m23 m7 m3c2
   ... the command in full is RESTORE
 LIQUID:L                FCC_A1                  BCC_A2
 GRAPHITE                SIGMA                   CEMENTITE
 M23C6                   M7C3                    M3C2
   RESTORED
TDB_FEDEMO: get
   ... the command in full is GET_DATA
15:40:01,257 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... 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) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
  'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C -Cr-Nb'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
      -C'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  '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'
  'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'P. Villars, L.D. Calvert. Pearsons handbook of crystallographic data for
      intermetallic phases, Metals park, Ohio 1985: American society for
      metals'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
      (2011) 479-491; Fe-Mn-C'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
TDB_FEDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: s-c t=1200,p=1e5,n=1 w(cr)=.13 w(c)=.01
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         10193 grid points in             1 s
```

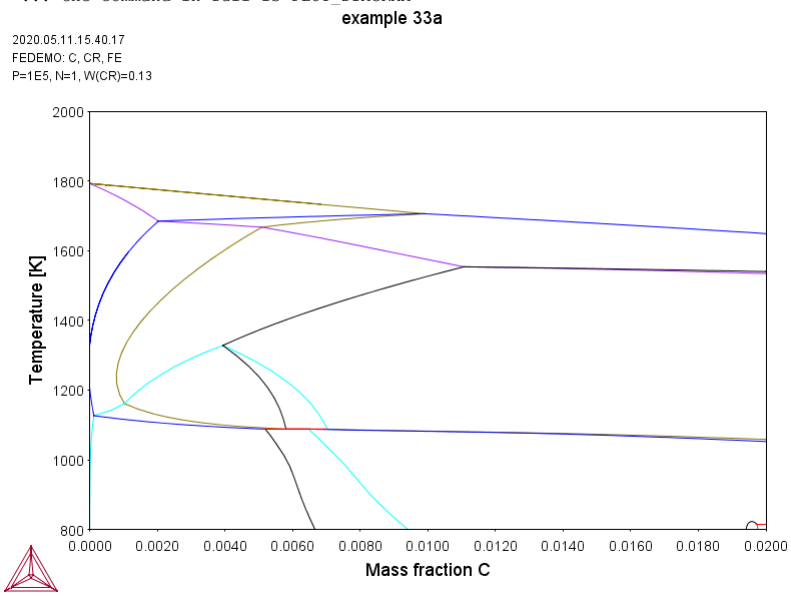
```
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     2  s
POLY: s-a-v 1 w(c) 0 .02
   ... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/: 5E-04
POLY: s-a-v 2 t 800 2000
   ... the command in full is SET_AXIS_VARIABLE
Increment /30/: 30
POLY: save tcex33 y
   ... the command in full is SAVE_WORKSPACES
POLY: 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:   6.615E-03  8.100E+02
     BCC_A2
     M23C6
  ** M7C3
 Calculated..                      2 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   6.665E-03  8.000E+02
     BCC_A2
     M23C6
  ** M7C3
 Calculated.                      11 equilibria

 Phase region boundary   3 at:   5.191E-03  1.088E+03
     BCC_A2
  ** FCC_A1#1
     M23C6
  ** M7C3

 Phase region boundary   4 at:   5.191E-03  1.088E+03
     BCC_A2
  ** FCC_A1#1
     M23C6
 Calculated.                      12 equilibria

 Phase region boundary   5 at:   1.203E-04  1.127E+03
     BCC_A2
  ** FCC_A1#1
  ** M23C6

 Phase region boundary   6 at:   1.203E-04  1.127E+03
     BCC_A2
  ** FCC_A1#1
 Calculated                      14 equilibria

 Phase region boundary   7 at:   1.203E-04  1.127E+03
     BCC_A2
  ** M23C6
 Calculated..                      12 equilibria
 Terminating at axis limit.

 Phase region boundary   8 at:   1.203E-04  1.127E+03
     BCC_A2
     FCC_A1#1
  ** M23C6
 Calculated.                       3 equilibria

 Phase region boundary   9 at:   1.027E-03  1.162E+03
  ** BCC_A2
     FCC_A1#1
  ** M23C6

 Phase region boundary  10 at:   1.027E-03  1.162E+03
     FCC_A1#1
  ** M23C6
```

```
Calculated.                      9 equilibria

Phase region boundary  11 at:   3.934E-03  1.328E+03
    FCC_A1#1
 ** M23C6
 ** M7C3

Phase region boundary  12 at:   3.934E-03  1.328E+03
    FCC_A1#1
 ** M23C6
    M7C3
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  13 at:   3.934E-03  1.328E+03
    FCC_A1#1
 ** M7C3
Calculated.                     19 equilibria

Phase region boundary  14 at:   1.106E-02  1.554E+03
 ** LIQUID
    FCC_A1#1
 ** M7C3

Phase region boundary  15 at:   1.106E-02  1.554E+03
    LIQUID
    FCC_A1#1
 ** M7C3
Calculated..                     20 equilibria
Terminating at axis limit.

Phase region boundary  16 at:   1.106E-02  1.554E+03
 ** LIQUID
    FCC_A1#1
Calculated.                     16 equilibria

Phase region boundary  17 at:   5.090E-03  1.667E+03
 ** LIQUID
 ** BCC_A2
    FCC_A1#1

Phase region boundary  18 at:   5.090E-03  1.667E+03
 ** LIQUID
    BCC_A2
    FCC_A1#1
Calculated.                      8 equilibria

Phase region boundary  19 at:   2.029E-03  1.685E+03
 ** LIQUID
    BCC_A2
 ** FCC_A1#1

Phase region boundary  20 at:   2.029E-03  1.685E+03
 ** LIQUID
    BCC_A2
Calculated                     23 equilibria

Phase region boundary  21 at:   2.029E-03  1.685E+03
    BCC_A2
 ** FCC_A1#1
Calculated                     26 equilibria

Phase region boundary  22 at:   2.029E-03  1.685E+03
    LIQUID
    BCC_A2
 ** FCC_A1#1
Calculated.                     17 equilibria

Phase region boundary  23 at:   9.895E-03  1.706E+03
    LIQUID
 ** BCC_A2
 ** FCC_A1#1

Phase region boundary  24 at:   9.895E-03  1.706E+03
    LIQUID
 ** FCC_A1#1
Calculated..                     22 equilibria
Terminating at axis limit.

Phase region boundary  25 at:   9.895E-03  1.706E+03
    LIQUID
 ** BCC_A2
Calculated                     32 equilibria

Phase region boundary  26 at:   9.895E-03  1.706E+03
    LIQUID
 ** BCC_A2
    FCC_A1#1
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   5.090E-03  1.667E+03
 ** BCC_A2
    FCC_A1#1
Calculated.                     18 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   1.106E-02  1.554E+03
 ** LIQUID
    FCC_A1#1
    M7C3
Calculated..                     20 equilibria
Terminating at axis limit.

Phase region boundary  29 at:   3.934E-03  1.328E+03
    FCC_A1#1
    M23C6
 ** M7C3
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   1.027E-03  1.162E+03
 ** BCC_A2
    FCC_A1#1
    M23C6
Calculated.                     14 equilibria
```

```
Terminating at known equilibrium

Phase region boundary  31 at:   6.464E-03  1.088E+03
    BCC_A2
 ** FCC_A1#1
    M7C3
Calculated..                     29 equilibria
Terminating at axis limit.

Phase region boundary  32 at:   7.028E-03  1.088E+03
 ** BCC_A2
    FCC_A1#1
    M7C3
Calculated..                     28 equilibria
Terminating at axis limit.

Phase region boundary  33 at:   6.464E-03  1.088E+03
    BCC_A2
 ** M23C6
    M7C3
Calculated..                     11 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  34 at:   6.615E-03  8.100E+02
    BCC_A2
    M23C6
 ** M7C3
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   5.000E-04  1.122E+03
    BCC_A2
 ** FCC_A1#1
    M23C6
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  36 at:   5.000E-04  1.122E+03
    BCC_A2
 ** FCC_A1#1
    M23C6
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   6.833E-03  1.055E+03
    BCC_A2
 ** M23C6
    M7C3
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  38 at:   6.833E-03  1.055E+03
    BCC_A2
 ** M23C6
    M7C3
Calculated..                     12 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  39 at:   1.317E-02  1.076E+03
    BCC_A2
 ** FCC_A1#1
    M7C3
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   1.317E-02  1.076E+03
    BCC_A2
 ** FCC_A1#1
    M7C3
Calculated..                     15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  41 at:   1.943E-02  8.100E+02
    BCC_A2
    M3C2
 ** M7C3
Calculated..                      3 equilibria
Terminating at axis limit.

Phase region boundary  42 at:   1.941E-02  8.000E+02
    BCC_A2
    M3C2
 ** M7C3
Calculated.                     19 equilibria

Phase region boundary  43 at:   1.973E-02  8.151E+02
    BCC_A2
 ** GRAPHITE
    M3C2
 ** M7C3

Phase region boundary  44 at:   1.973E-02  8.151E+02
    BCC_A2
 ** GRAPHITE
    M3C2
Calculated..                      2 equilibria
Terminating at axis limit.

Phase region boundary  45 at:   2.266E-02  8.151E+02
    BCC_A2
 ** GRAPHITE
    M7C3

Phase region boundary  46 at:   7.607E-01  8.151E+02
 ** BCC_A2
    GRAPHITE
    M7C3

Phase region boundary  47 at:   2.266E-02  8.151E+02
    BCC_A2
 ** M3C2
    M7C3
```

```
Phase region boundary  48 at:   7.607E-01  8.151E+02
    GRAPHITE
 ** M3C2
    M7C3

Phase region boundary  49 at:   1.943E-02  8.100E+02
    BCC_A2
    M3C2
 ** M7C3
Calculated.                     22 equilibria
Terminating at known equilibrium

Phase region boundary  50 at:   1.950E-02  8.204E+02
    BCC_A2
    M3C2
 ** M7C3
Calculated..                     7 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  51 at:   1.950E-02  8.204E+02
    BCC_A2
    M3C2
 ** M7C3
Calculated.                      8 equilibria
Terminating at known equilibrium

Phase region boundary  52 at:   8.289E-04  1.203E+03
 ** BCC_A2
    FCC_A1#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  53 at:   8.289E-04  1.203E+03
 ** BCC_A2
    FCC_A1#1
Calculated.                     17 equilibria
Terminating at known equilibrium

Phase region boundary  54 at:   6.104E-03  1.203E+03
    FCC_A1#1
 ** M23C6
    M7C3
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary  55 at:   6.104E-03  1.203E+03
    FCC_A1#1
 ** M23C6
    M7C3
Calculated.                      7 equilibria
Terminating at known equilibrium

Phase region boundary  56 at:   1.148E-03  1.597E+03
    BCC_A2
 ** FCC_A1#1
Calculated                     26 equilibria

Phase region boundary  57 at:   1.148E-03  1.597E+03
    BCC_A2
 ** FCC_A1#1
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  58 at:   8.870E-03  1.597E+03
 ** LIQUID
    FCC_A1#1
Calculated.                      7 equilibria
Terminating at known equilibrium

Phase region boundary  59 at:   8.870E-03  1.597E+03
 ** LIQUID
    FCC_A1#1
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  60 at:   5.000E-04  1.788E+03
    LIQUID
 ** BCC_A2
Calculated                     22 equilibria

Phase region boundary  61 at:   5.000E-04  1.788E+03
    LIQUID
 ** BCC_A2
Calculated.                     20 equilibria
Terminating at known equilibrium

Phase region boundary  62 at:   6.833E-03  1.733E+03
    LIQUID
 ** BCC_A2
Calculated                     26 equilibria

Phase region boundary  63 at:   6.833E-03  1.733E+03
    LIQUID
 ** BCC_A2
Calculated.                      8 equilibria
Terminating at known equilibrium

Phase region boundary  64 at:   1.317E-02  1.688E+03
    LIQUID
 ** FCC_A1#1
Calculated.                      8 equilibria
Terminating at known equilibrium

Phase region boundary  65 at:   1.317E-02  1.688E+03
    LIQUID
 ** FCC_A1#1
Calculated..                     15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  66 at:   1.950E-02  1.652E+03
    LIQUID
 ** FCC_A1#1
Calculated.                     21 equilibria
Terminating at known equilibrium
```

```
 Phase region boundary  67 at:   1.950E-02  1.652E+03
     LIQUID
  ** FCC_A1#1
 Calculated..                       3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex33\tcex33.POLY3
 CPU time for mapping                     8 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST: set-title example 33a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

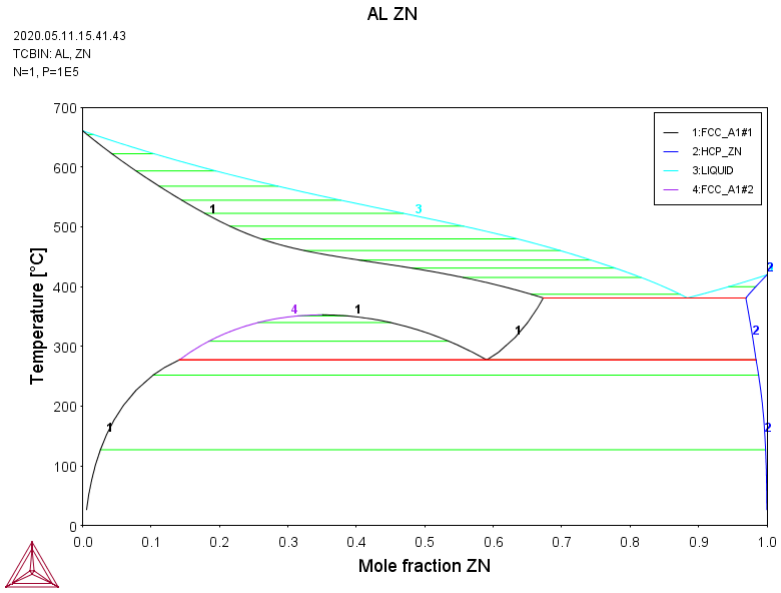



```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

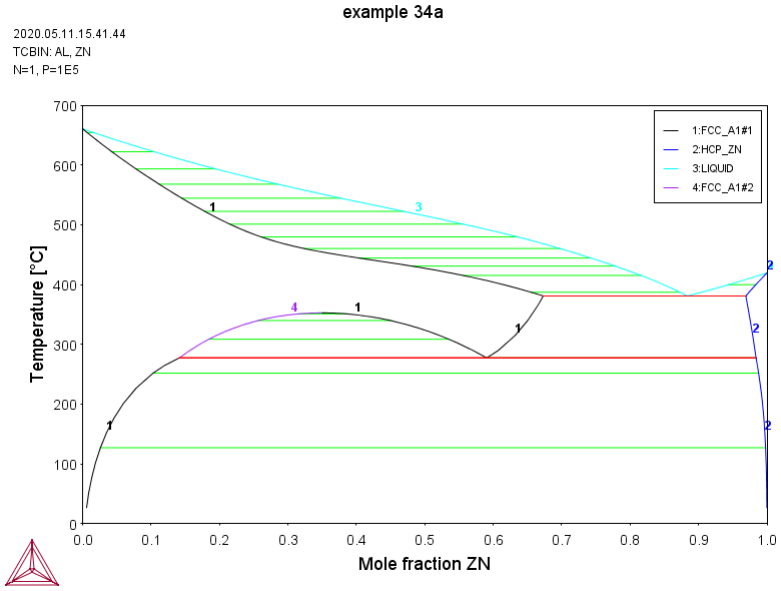
tcex34

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex34\tcex34.TCM"
SYS: set-echo
SYS:
SYS: @@ The Al-Zn phase diagram and its G curve
SYS:
SYS: @@ This example uses the BINARYÂ module to calculate
SYS: @@ the phase diagram and G curves in the Al-Zn system.
SYS:
SYS: go bin
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC  Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase_Diagram
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES .....
 AL                      ZN  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  TETRAGONAL_A6           RHOMBOHEDRAL_A7
 CBCC_A12                CUB_A13                 B32_ALLI
 B3_ZINCBLENDE           C14_LAVES               C15_LAVES
 C16_AL2CU               C36_LAVES               D019_AL1M3
 D513_AL3NI2             D82_FEZN_GAMMA          L10_ALTI
 AGZN_ZETA               AL5FE4                  ALCE_AMORPHOUS
 ALCU_ETA                FEZN4                   FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 HCP_ZN  RESTORED
15:41:37,332 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
 -OK-
 Creating a new composition set FCC_A1#2
 The condition X(ZN)=.1234  created
 The condition T=612.43  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
 Start points provided by database
 Version S mapping is selected

 Organizing start points

 Generating start point   1
 Generating start point   2

 Phase region boundary   1 at:   5.345E-01  5.000E+02
  ** FCC_A1#1
     HCP_ZN
 Calculated..                     10 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:   5.027E-01  3.000E+02
  ** FCC_A1#1
     HCP_ZN
 Calculated.                     13 equilibria

 Phase region boundary   3 at:   5.626E-01  5.504E+02
  ** FCC_A1#1
  ** FCC_A1#2
     HCP_ZN

 Phase region boundary   4 at:   7.872E-01  5.504E+02
  ** FCC_A1#1
     HCP_ZN
 Calculated.                      6 equilibria
```

```
 Phase region boundary   5 at:   8.211E-01  6.540E+02
  ** LIQUID
  ** FCC_A1#1
     HCP_ZN

 Phase region boundary   6 at:   9.263E-01  6.540E+02
  ** LIQUID
     HCP_ZN
 Calculated                     17 equilibria

 Phase region boundary   7 at:   7.783E-01  6.540E+02
  ** LIQUID
     FCC_A1#1
 Calculated                     73 equilibria

 Phase region boundary   8 at:   3.658E-01  5.504E+02
  ** FCC_A1#1
     FCC_A1#2
 Calculated                     28 equilibria

 Phase region boundary   9 at:   5.345E-01  5.000E+02
  ** FCC_A1#1
     HCP_ZN
 Calculated.                     5 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: C:\Users\vagrant\AppData\Local\Temp\BINARY_002.POLY3
 CPU time for mapping                        2 seconds
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes
```

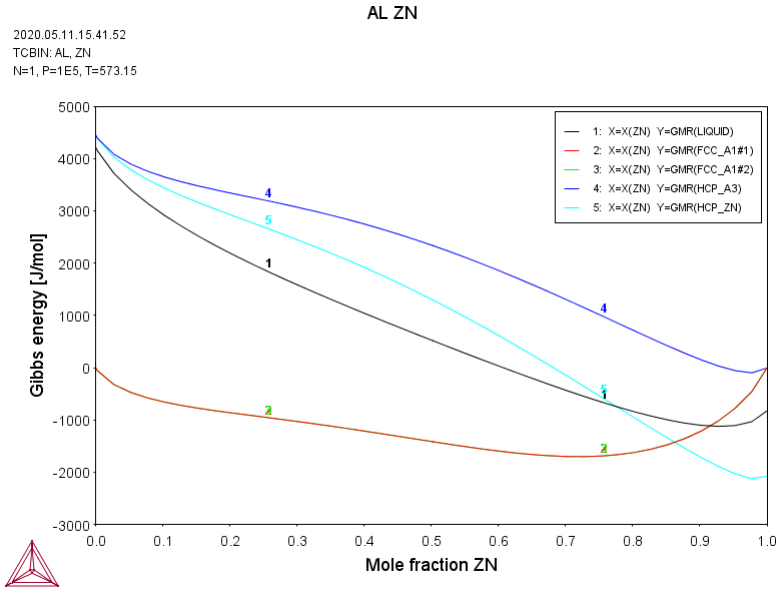



```
POST: set-title example 34a
POST: plot
```

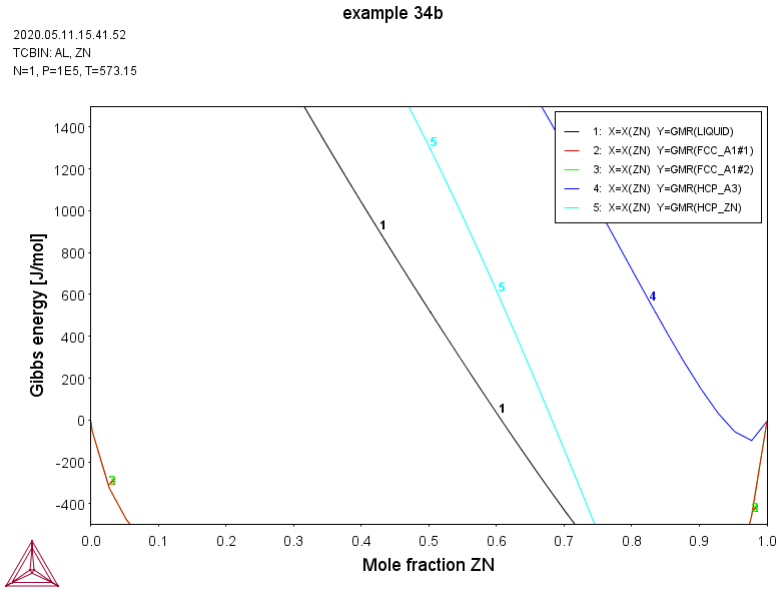



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot a G curve at 573 K!
POST: back
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
SYS: go bin
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
```

```
 DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC  Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G
Temperature (C): /1000/: 300
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES .....
 AL                      ZN  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  TETRAGONAL_A6           RHOMBOHEDRAL_A7
 CBCC_A12                CUB_A13                 B32_ALLI
 B3_ZINCBLENDE           C14_LAVES               C15_LAVES
 C16_AL2CU               C36_LAVES               D019_AL1M3
 D513_AL3NI2             D82_FEZN_GAMMA          L10_ALTI
 AGZN_ZETA               AL5FE4                  ALCE_AMORPHOUS
 ALCU_ETA                FEZN4                   FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 HCP_ZN  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
 -OK-
 Creating a new composition set FCC_A1#2
 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

 Phase Region from   0.502463     for:
     LIQUID
     FCC_A1#1
     FCC_A1#2
     HCP_A3
     HCP_ZN

 Phase Region from   0.502463     for:
     LIQUID
     FCC_A1#1
     FCC_A1#2
     HCP_A3
     HCP_ZN
*** Buffer saved on file *** C:\Users\vagrant\AppData\Local\Temp\GCURVE_002.POLY3
 POSTPROCESSOR VERSION 3.2
```

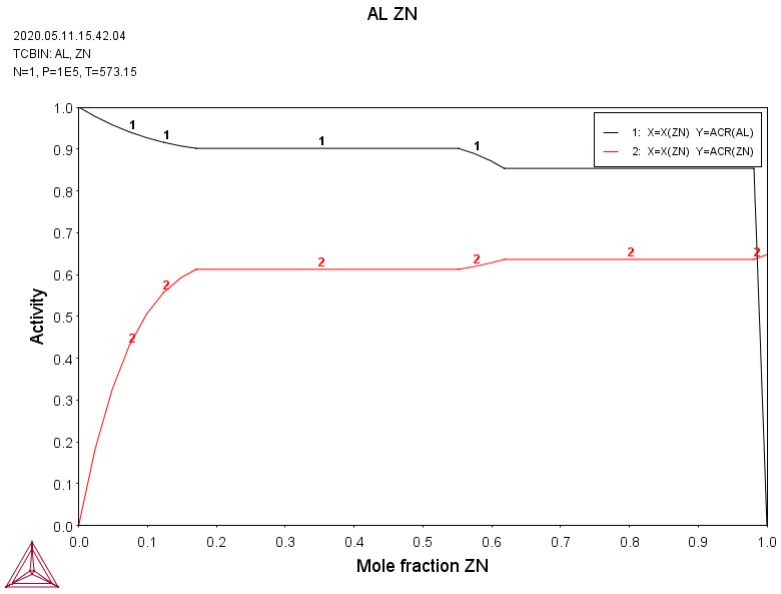



```
POST: s-s y n -500 1500
POST:
POST: set-title example 34b
POST:
POST: plot
```

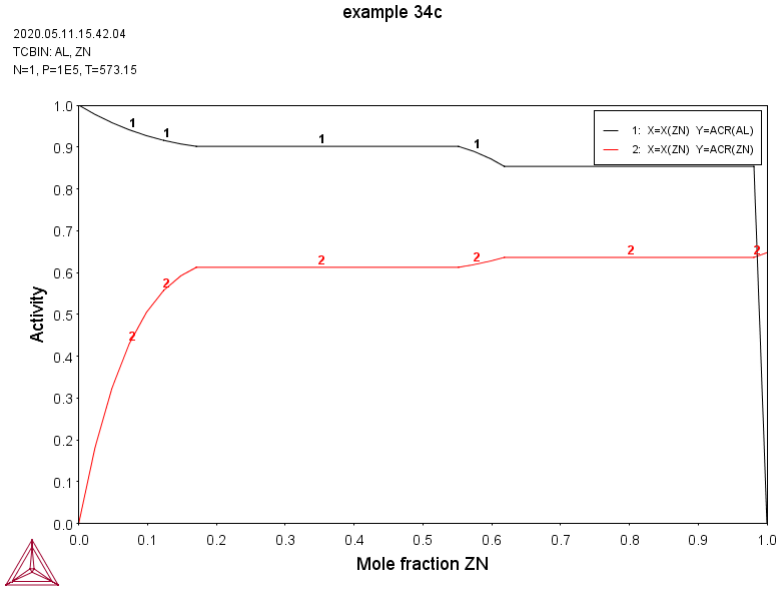



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot an activity (A) curve at 573 K
POST: back
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
SYS: go bin
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC  Binary Solutions  v1.1

 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: A
Temperature (C): /1000/: 300
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES .....
 AL                      ZN  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  TETRAGONAL_A6           RHOMBOHEDRAL_A7
 CBCC_A12                CUB_A13                 B32_ALLI
 B3_ZINCBLENDE           C14_LAVES               C15_LAVES
 C16_AL2CU               C36_LAVES               D019_AL1M3
 D513_AL3NI2             D82_FEZN_GAMMA          L10_ALTI
 AGZN_ZETA               AL5FE4                  ALCE_AMORPHOUS
 ALCU_ETA                FEZN4                   FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 HCP_ZN  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
 -OK-
 Creating a new composition set FCC_A1#2
 The condition X(ZN)=.1234  created

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

 Forcing automatic start values
 Automatic start values will be set
 No initial equilibrium, using default
 Step will start from axis value   0.123400
...OK

 Phase Region from   0.123400     for:
     FCC_A1#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_ZN
 Global test at  7.98400E-01 .... OK
 Global check of removing phase at  9.81102E-01
 Calculated    18 equilibria

 Phase Region from   0.981102     for:
     HCP_ZN
 Terminating at    1.00000
 Calculated     4 equilibria

 Phase Region from   0.123400     for:
     FCC_A1#1
 Terminating at   0.100000E-11
 Calculated     8 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\GCURVE_002.POLY3
  POSTPROCESSOR VERSION 3.2
```

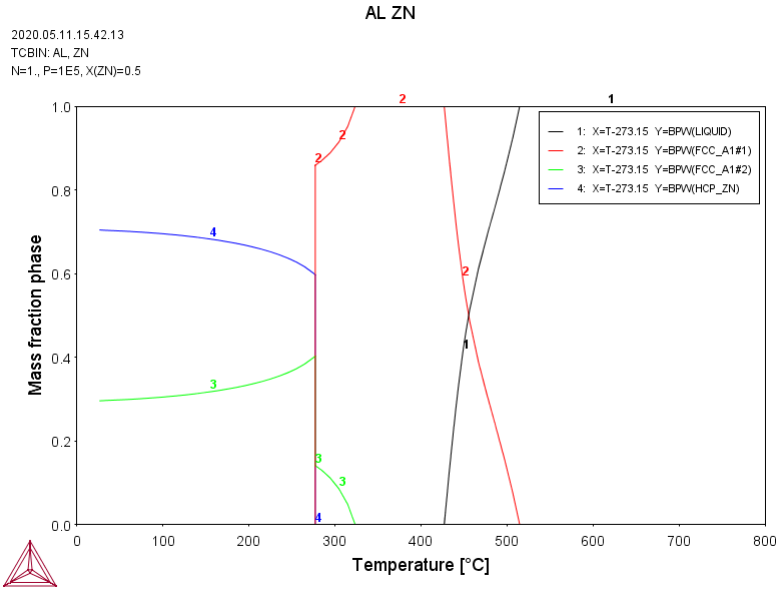



```
POST:
POST: set-title example 34c
POST:
POST: plot
```

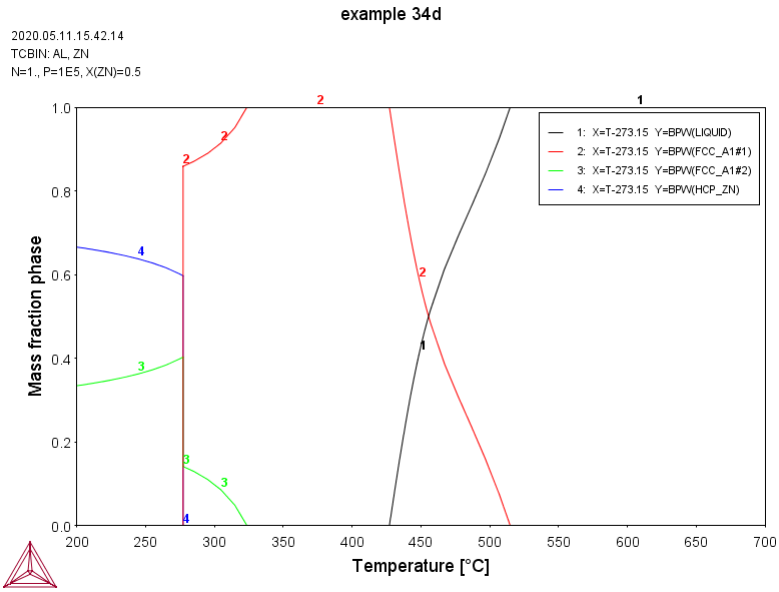



```
POST:
POST:Hit RETURN to continue
POST: @@ Now plot a Phase fraction (F) curve for
POST: @@ x(zn)=.5. The miscibility gap is found now
POST: back
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
SYS: go bin
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED

 Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
 Current database: TC  Binary Solutions  v1.1
```

```
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: F
Fraction of: zn /.5/: .5
 VA                      /-  DEFINED
 BCC_B2                  FCC_L12                 FCC_L102
 D021_HCP  REJECTED
 REINITIATING GES .....
 AL                      ZN  DEFINED
 GAS:G                   LIQUID:L                IONIC_LIQUID:Y
 FCC_A1                  BCC_A2                  A2_BCC
 HCP_A3                  HCP_ZN                  DIAMOND_A4
 BCT_A5                  TETRAGONAL_A6           RHOMBOHEDRAL_A7
 CBCC_A12                CUB_A13                 B32_ALLI
 B3_ZINCBLENDE           C14_LAVES               C15_LAVES
 C16_AL2CU               C36_LAVES               D019_AL1M3
 D513_AL3NI2             D82_FEZN_GAMMA          L10_ALTI
 AGZN_ZETA               AL5FE4                  ALCE_AMORPHOUS
 ALCU_ETA                FEZN4                   FEZN_DELTA
 FEZN_ZETA  REJECTED
 LIQUID:L  RESTORED
 FCC_A1  RESTORED
 HCP_A3  RESTORED
 HCP_ZN  RESTORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
  'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
  'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
 -OK-
 Creating a new composition set FCC_A1#2

 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    1000.00
...OK

 Phase Region from    1000.00     for:
     LIQUID
 Global test at  9.20000E+02 .... OK
 Global test at  8.20000E+02 .... OK
 Global check of adding phase at  7.88048E+02
 Calculated    24 equilibria

 Phase Region from    788.048     for:
     LIQUID
     FCC_A1#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_ZN
 Calculated     2 equilibria

 Phase Region from    550.386     for:
     FCC_A1#2
     HCP_ZN
 Global test at  4.78000E+02 .... OK
 Global test at  3.78000E+02 .... OK
 Terminating at    300.000
 Calculated    29 equilibria
 *** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\PFCURVE_002.POLY3
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes
```




```
POST:
POST: s-s x n 200 700
POST: set-title example 34d
POST:
POST: plot
```



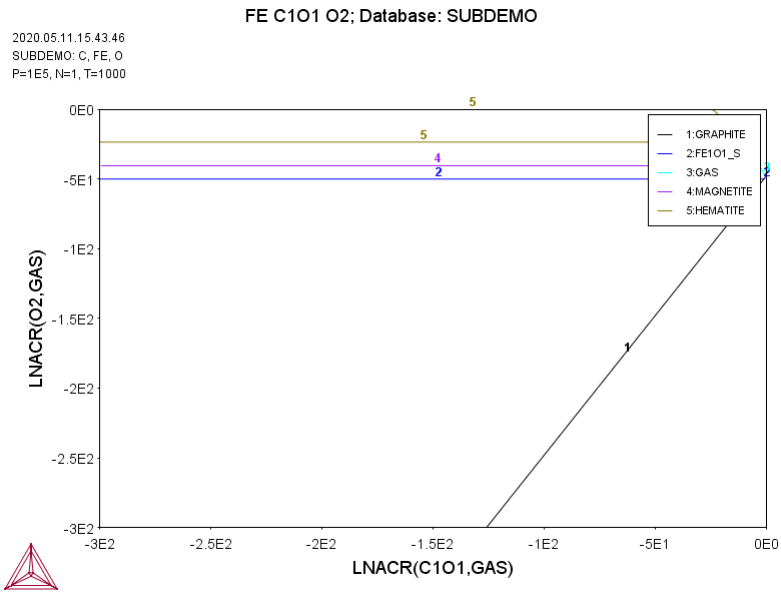

```
POST:
POST: set-inter
POST:
```

tcex35

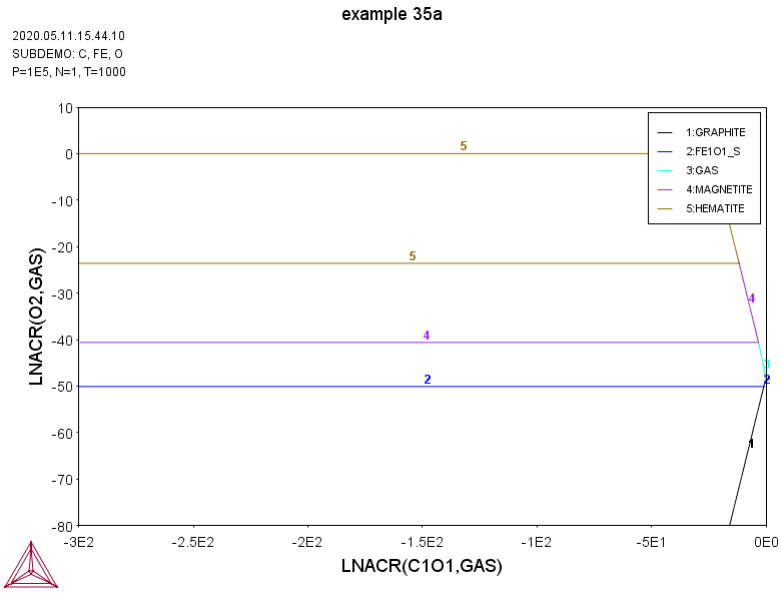
```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex35\tcex35.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating a potential diagram using
SYS: @@ the POTENTIALÃ module.
SYS:
SYS: @@ There are no commands for this module, you
SYS: @@ just follow the prompts.
SYS:
SYS: go pot

 Simple potential phase diagram calculation module

Database: /POT/: SUBDEMO
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Substance Demo Database v1.0

 VA                      /-  DEFINED
Matrix element: /FE/: FE
First potential species: /S1O2/: C1O1
Second potential species: /O2/: O2
Temperature: /1000/: 1000
 VA                      /-  DEFINED
 REINITIATING GES .....
 FE                      C                       O
   DEFINED
15:43:31,430 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'C1<G> T.C.R.A.S. Class: 1 C1<G> C<G>'
  'C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE ** C1O1<G> CO<G> CARBON MONOXIDE
      <GAS> STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65'
  'C1O2<G> T.C.R.A.S. Class: 2 C1O2<G> CO2<G> CARBON DIOXIDE <GAS>'
  'C2<G> T.C.R.A.S. Class: 2 C2<G> CARBON Diatomic Gas.'
  'C2O1<G> T.C.R.A.S. Class: 5 C2O1<G> C2O<G>'
  'C3<G> T.C.R.A.S. Class: 6 C3<G> CARBON <TRIATOMIC GAS>'
  'C3O2<G> T.C.R.A.S. Class: 6 C3O2<G>'
  'C4<G> T.C.R.A.S. Class: 7 C4<G>'
  'C5<G> T.C.R.A.S. Class: 7 C5<G>'
  'C5FE1O5<G> JANAF 1982 SGTE C5FE1O5<G> Fe(CO)5<G> IRON PENTACARBONYL <GAS>
      ASSESSMENT DATED 3/78'
  'C60<G> MHR-95 C60<G> Data processed from [94Kor/Sid] M.V. Korobov, L.N.
      sidorov, J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the
      rotational data in [91McK] and vibration frequencies in [94Kor/Sid].
      Note that a frequency with degeneracy 5 is missing from list in
      [94Kor/Sid]; taken to be 419 cm-1, which gives very good, though not
      exact, agreement with values quoted in [94Kor/Sid]. Note discrepancy
      between calculated DrS(298) = -8943.5 J mol K-1 for the reaction 60C<g>
      =C60<g>and that given by [94Kor/Sid] in their Table 5, -8950 J mol K
      -1. Enthalpy of formation: DfH = 2588 kJ/mol from DsubH(298.15K) = 166
      +/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure values reproduced very
      well. [91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).'
  'FE1<G> THERMODATA FE1<G> Fe<G> Data provided by T.C.R.A.S. October 1996
      Modified by Thermodata - new assessment'
  'FE1O1<G> TCRAS 5-F FEO IRON OXIDE 23/11/06 FE1O1<G> FeO<G>'
  'FE1O2<G> T.C.R.A.S Class: 6 FE1O2<G> FeO2<G> Data provided by TCRAS.
      October 1996. Error in version 1997. S298 corrected to 1bar 20080222
      AAZ TCRAS2006 : dH, S'
  'FE2<G> THERMODATA FE2<G> Fe2<G> Data provided by T.C.R.A.S. October 1996
      Modified by Thermodata - new assessment. Typing error corrected 12/06'
  'O2<G> TCRAS 21/06/90 O2<G> OXYGEN Gaseous Standard State.'
  'O3<G> TCRAS 02/06/80 O3<G> OZONE Gaseous Standard State.'
  'C1FE1O3 N.P.L. SGTE ** C1FE1O3 FeCO3 Siderite IRON<2> CARBONATE
      DECOMPOSES BEFORE FUSION.'
  'C1FE3 N.P.L. SGTE ** C1FE3 Fe3C Cementite CEMENTITE'
  'C5FE1O5<L> I. BARIN 3rd. Edition C5FE1O5_Liquid Fe(CO)5_Liquid IRON
      PENTACARBONYL (Liquid). Same as in previous versions. Rounding of H298.'
  'C60 MHR-95 C60 Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov,
       J. Chem. The Fitted to the data in [94Kor/Sid], who took the phase
      transition at 257K that [94Kor/Sid] do not give an explicit value for
      S(298.15K). S(298.15K) = 422.6 J mol K-1 was calculated from S(300) =
      425.8 and Cp e calculated from DrS(298) for 60C<graphite>=C60 given by
      [94Kor/Sid] in their Table 5, which gives S(298.15K) = 425.4 J mol K
      -1. Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],
       the value preferred, if obliquely, by [94Kor/Sid]. [92Ste/Chi]W.V.
      Steele, R.D. Chirico, N.K. Smith, W.e. Billups, P.R. Elmore, A.E.
      Wheeler, J. Phys. Chem. 96 4731 (1993).'
  'C1<DIAMOND> S.G.T.E. ** C_DIAMOND <DIAMOND> Data from SGTE Unary DB, data
      added by atd 7/9/95, H298-H0 taken from 1994 database (ex THERMODATA
      01/93)'
  'FE1O1 T.C.R.A.S Class: 5 FE1O1 FeO FeO_Wustite IRON OXIDE. Data provided
      by T.C.R.A.S. in 2000'
  'FE2O3<FE2O3_GAMMA> T.C.R.A.S Class: 5 FE2O3_GAMMA Fe2O3_Gamma Data
      provided by T.C.R.A.S. in 2000'
  'FE1 S.G.T.E. ** FE1 Fe Data from SGTE Unary DB'
  'C1<GRAPHITE> S.G.T.E. ** C_GRAPHITE Data from SGTE Unary DB, pressure
      dependent data added by atd 7/9/95'
  'FE2O3<HEMATITE> T.C.R.A.S Class: 7 FE2O3 Fe2O3 Hematite Data provided by
      T.C.R.A.S. in 2000 with previous description of the magnetic
      transition fitted by IA. In version 2000 only H298 has been changed.'
  'FE3O4<MAGNETITE> JANAF 4th Ed. FE3O4 Fe3O4 MAGNETITE Data refitted by IA
```

```
     to reproduce the magnetic transition.'
 'FE0.947O1<WUSTITE> T.C.R.A.S Class: 5 FE0.947O1 Fe0.947O WUSTITE WUSTITE.
     Data provided by T.C.R.A.S. in 2000 20080222 AAZ TCRAS2006 : dH, S'
-OK-
This command is DEPRECATED and to be removed in the future!
Please use ADVANCED_OPTIONS instead of SPECIAL_OPTIONS
The condition LNACR(C1O1,GAS)=-140.8589  created
The condition LNACR(O2,GAS)=-140.8589  created
Normal POLY minimization, not global
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

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

Phase region boundary   1 at:  -4.633E+01 -1.409E+02
    FE_S
 ** GRAPHITE
Calculated..                     81 equilibria
Terminating at axis limit.

Phase region boundary   2 at:  -1.259E+02 -3.000E+02
    FE_S
 ** GRAPHITE
Calculated.                     126 equilibria

Phase region boundary   3 at:  -9.383E-01 -5.007E+01
 ** FE1O1_S
    FE_S
 ** GRAPHITE

Phase region boundary   4 at:  -9.383E-01 -5.007E+01
 ** FE1O1_S
    FE_S
Calculated..                    151 equilibria
Terminating at axis limit.

Phase region boundary   5 at:  -9.383E-01 -5.007E+01
 ** FE1O1_S
    GRAPHITE
Calculated.                      2 equilibria

Phase region boundary   6 at:  -3.398E-01 -4.887E+01
 ** GAS
 ** FE1O1_S
    GRAPHITE

Phase region boundary   7 at:  -3.398E-01 -4.887E+01
 ** GAS
    GRAPHITE
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Phase region boundary   8 at:  -3.398E-01 -4.887E+01
 ** GAS
    FE1O1_S
Calculated.                      7 equilibria

Phase region boundary   9 at:  -3.272E+00 -4.059E+01
 ** GAS
    FE1O1_S
 ** MAGNETITE

Phase region boundary  10 at:  -3.272E+00 -4.059E+01
    FE1O1_S
 ** MAGNETITE
Calculated..                    150 equilibria
Terminating at axis limit.

Phase region boundary  11 at:  -3.272E+00 -4.059E+01
    GAS
 ** MAGNETITE
Calculated.                     10 equilibria

Phase region boundary  12 at:  -1.174E+01 -2.359E+01
    GAS
 ** HEMATITE
 ** MAGNETITE

Phase region boundary  13 at:  -1.174E+01 -2.359E+01
    GAS
 ** HEMATITE
Calculated..                    168 equilibria
Terminating at axis limit.

Phase region boundary  14 at:  -1.174E+01 -2.359E+01
 ** HEMATITE
    MAGNETITE
Calculated..                    146 equilibria
Terminating at axis limit.

Phase region boundary  15 at:  -4.633E+01 -1.409E+02
    FE_S
 ** GRAPHITE
Calculated.                     47 equilibria
Terminating at known equilibrium

Phase region boundary  16 at:  -1.409E+02 -5.007E+01
 ** FE1O1_S
    FE_S
Calculated..                     81 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  17 at:  -1.409E+02 -5.007E+01
 ** FE1O1_S
    FE_S
Calculated.                     71 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex35\POT.POLY3
CPU time for mapping                     5 seconds
```

```
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes
```




```
POST: s-s y n -80 10
POST: set-title example 35a
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```




```
POST:
POST: set-inter
POST:
```

tcex36a

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36a.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Assessment. The use of the PARROT module
SYS:
SYS: @@ This is the setup file for Windows systems
SYS:
SYS: @@ First the elements and phases must be entered in G-E-S module
SYS: GO G
 GIBBS ENERGY SYSTEM
15:45:26,673 INFO  *** Invoking Gibbs Energy System v6 ***
GES: ENTER-ELEMENT A B
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 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
 Creating a new composition set BCC#2
GES: @@ We can also set the major constituent of the first composition set
GES: AMEND_PHASE BCC MAJOR 1 A
GES:
GES: @@ The FCC phase is stable only for element B
GES: AMEND_PHASE FCC MAJOR 1 B
GES: @@ The parameters can be entered in the PARROT module
GES: GO PAR

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: ENTER-PARAMETER G(BCC,A) 500 0; 2000 N
 G(BCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(BCC,B) 500 0; 2000 N
 G(BCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A) 500 14000-10*T; 2000 N
 G(LIQUID,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(LIQUID,B) 500 18000-12*T; 2000 N
 G(LIQUID,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,B) 500 3300-3*T; 2000 N
 G(FCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,A) 500 408; 2000 N
 G(FCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(A2B) 500 V1+V2*T+V3*T*LOG(T); 2000 N
 G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;0) 500 V11+V12*T; 2000 N
 G(LIQUID,A,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;1) 500 V13+V14*T; 2000 N
 G(LIQUID,A,B;1)
PARROT: ENTER-PARAMETER G(BCC,A,B;0) 500 V15+V16*T; 2000 N
 G(BCC,A,B;0)
PARROT: ENTER-PARAMETER G(BCC,A,B;1) 500 V17+V18*T; 2000 N
 G(BCC,A,B;1)
PARROT: ENTER-PARAMETER G(FCC,A,B;0) 500 V19+V20*T; 2000 N
 G(FCC,A,B;0)
PARROT: ENTER-PARAMETER G(FCC,A,B;1) 500 V21+V22*T; 2000 N
 G(FCC,A,B;1)
PARROT:
PARROT: @@ Everything is saved to an unformatted work file by the Create command
PARROT: CREATE tcex36
PARROT:
PARROT:Hit RETURN to continue
PARROT:
PARROT: @@ The experimental data file is compiled to the work file.
PARROT: COMPILE tcex36 screen Y exp36
POP files may include graphics information using the
GRAPHICS_PLOT command. A file name for generating an ".exp" file must be given.
 $
 $ POP file for assessment example
 $
 $ Enter some constants used later.
 ENTER_SYMBOL CONSTANT  DX=0.02,P0=101325,DH=500,DT=10
 $
 $ Eutectic point at A rich side from ref #2.
 $ T=1193 K, 40.8 w/o B in liquid, 13 w/o B in bcc.
 $ In a binary system one must have four conditions if P is not fixed.
 $ We obtain this by fixing the pressure and that three phases must be stable.
 $ The amount of the fixed phases is irrelevant here
 CREATE_NEW_EQUILIBRIUM 1,1
 CHANGE_STATUS PHASE LIQUID,BCC,A2B=FIX 1
 SET-CONDITION P=P0
 EXPERIMENT  T=1193:DT,W(LIQ,B)=.408:DX,W(BCC,B)=.13:DX
 GRAPHICS 1 .408 1193 MS5
 GRAPHICS 1 .13  1193 DS5
 GRAPHICS 1 .555 1193 DS5
 LABEL AINV
 SET-ALT X(A2B,A)=.6666667
```

```
SET_ALL_START  1193 Y
Automatic start values will be set
$
$ Congrent melting temperature for A2B 1341 K.
$ We will include the enthalpy of transformation also and this
$ requires a function.
ENTER_SYMBOL FUNCTION  HTR=HM(LIQUID)-HM(A2B);
$
$ Note how one specifies that this is a congruent transformation!
CREATE_NEW_EQUILIBRIUM 2,1
CHANGE_STATUS PHASE LIQ,A2B=FIX 1
SET-CONDITION P=P0,X(LIQ,B)-X(A2B,B)=0
EXPERIMENT  T=1341:DT
EXPERIMENT  HTR=3727:500
GRAPHICS 1 .555 1341 MS7
LABEL AINV
SET-ALT X(A)=.6666667
SET_ALL_START  1341 Y
Automatic start values will be set
$
$ Eutectic point at B rich side.
$ T=1049 K, 27 w/o A in liquid, 9.3 w/o A in bcc.
CREATE_NEW_EQUILIBRIUM 3,1
CHANGE_STATUS PHASE LIQ,BCC,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT  T=1049:DT,W(LIQ,A)=.27:DX,W(BCC,A)=.093:DX
SET-ALT X(A2B,A)=.66666667
GRAPHICS 1 .907 1049 MS5
GRAPHICS 1 .73  1049 DS5
GRAPHICS 1 .555 1049 DS5
LABEL AINV
SET_ALL_START  1049 Y
Automatic start values will be set
$
$ Peritectic point. T=1203 K, 19 w/o A in liquid, 6.9 w/o A in bcc,
$ 6.0 w/o A in fcc.
CREATE_NEW_EQUILIBRIUM 4,1
CHANGE_STATUS PHASE LIQ,BCC,FCC=FIX 1
SET-CONDITION P=P0
EXPERIMENT  T=1203:DT,W(LIQ,A)=.19:DX,W(BCC,A)=.069:DX,W(FCC,A)=.06:DX
GRAPHICS 1 .81 1203 MS5
GRAPHICS 1 .931 1203 DS5
GRAPHICS 1 .94 1203 DS5
LABEL AINV
SET_ALL_START  1203 Y
Automatic start values will be set
$
$ Eutectoid transformation of A2B -> BCC1 + BCC2, from ref #3
$ T=726, 3.7 at/o B in A, 11.4 at/o A in B
$ Note that miscibility gaps are indicated by using # after the phase
$ name and then give an integer.
CREATE_NEW_EQUILIBRIUM 5,1
CHANGE_STATUS PHASE BCC#1,BCC#2,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT  T=726:DT,X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
SET-ALT X(A2B,A)=.6666667
GRAPHICS 1 0.09 726 MS5
GRAPHICS 1 0.95 726 DS5
LABEL AINV
SET_ALL_START  726 Y
Automatic start values will be set
$
$ It is sometimes useful to decribe an invariant equilibria as
$ three tie-lines between each pair of phases at the same temperature.
$ In this case it helps to add a tie-line across the miscibility gap
$ at the invariant temperature.
CREATE_NEW_EQUILIBRIUM 6,1
CHANGE_STATUS PHASE BCC#1,BCC#2=FIX 1
SET-CONDITION P=P0 T=726
EXPERIMENT  X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
LABEL AINV
SET_ALL_START Y
Automatic start values will be set
$
$ From ref #4 the liquidus at the B rich end:
$ The table values are referenced inside the table_head using @<column>
TABLE_HEAD 10
CREATE_NEW_EQUILIBRIUM 0010,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1594,P=P0
EXPERIMENT  W(LIQ,A)=0.02:DX
LABEL ALF
GRAPHICS 1 .98 1594 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0011,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1548,P=P0
EXPERIMENT  W(LIQ,A)=0.042:DX
LABEL ALF
GRAPHICS 1 .958 1548 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0012,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1499,P=P0
EXPERIMENT  W(LIQ,A)=0.065:DX
LABEL ALF
GRAPHICS 1 .935 1499 MS5
SET_ALL_START Y
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0013,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1438,P=P0
EXPERIMENT  W(LIQ,A)=0.093:DX
LABEL ALF
GRAPHICS 1 .907 1438 MS5
SET_ALL_START Y
Automatic start values will be set

$
$ From ref #5 we have the following tie-lines
TABLE_HEAD 20
CREATE_NEW_EQUILIBRIUM 0020,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1413,P=P0
```

```
EXPERIMENT  W(LIQ,A)=.104:DX,W(FCC,A)=.038:DX
GRAPHICS 1 .896 1413 MS9
GRAPHICS 1 .962 1413 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE  Y(LIQ,A)=.104,Y(FCC,A)=.038
CREATE_NEW_EQUILIBRIUM 0021,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1337,P=P0
EXPERIMENT  W(LIQ,A)=.136:DX,W(FCC,A)=.047:DX
GRAPHICS 1 .864 1337 MS9
GRAPHICS 1 .953 1337 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE  Y(LIQ,A)=.136,Y(FCC,A)=.047
CREATE_NEW_EQUILIBRIUM 0022,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1213,P=P0
EXPERIMENT  W(LIQ,A)=.187:DX,W(FCC,A)=.059:DX
GRAPHICS 1 .813 1213 MS9
GRAPHICS 1 .941 1213 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE  Y(LIQ,A)=.187,Y(FCC,A)=.059
CREATE_NEW_EQUILIBRIUM 0023,1
CHANGE_STATUS PHASE LIQ,BCC=FIX 1
SET-CONDITION T=1100,P=P0
EXPERIMENT  W(LIQ,A)=.245:DX,W(BCC,A)=.085:DX
GRAPHICS 1 .755 1100 MS9
GRAPHICS 1 .915 1100 DS9
LABEL ATIE
SET_ALL_START Y
Automatic start values will be set
SET_START_VALUE  Y(LIQ,A)=.245,Y(BCC,A)=.085

$
$ Thermochemical data
$ Activities of B in liquid (reference state fcc) at 1573 K.
$ The command SET_REFERENCE_STATE is used for this as the default
$ reference state for B is BCC.
$
$ Note that we have set an uncertainity on the fraction (condition) also.
TABLE_HEAD 100
CREATE_NEW_EQUILIBRIUM 0100,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.90:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.94:DX
GRAPHICS 3 .90 .94 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0101,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.80:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.84:DX
GRAPHICS 3 .80 .84 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0102,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.70:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.74:DX
GRAPHICS 3 .70 .74 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0103,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.60:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.64:DX
GRAPHICS 3 .60 .64 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0104,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.50:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.54:DX
GRAPHICS 3 .50 .54 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0105,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.40:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.44:DX
GRAPHICS 3 .40 .44 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0106,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.30:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.34:DX
GRAPHICS 3 .30 .34 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0107,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.20:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.23:DX
GRAPHICS 3 .20 .23 MS1
LABEL AA
CREATE_NEW_EQUILIBRIUM 0108,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.10:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.12:DX
GRAPHICS 3 .10 .12 MS1
LABEL AA

$
$ Enthalpy of mixing at 1773 K (reference state: liquid)
TABLE_HEAD 110
CREATE_NEW_EQUILIBRIUM 0110,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.9
```

```
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-1964:DH
 GRAPHICS 2 .9 -1964 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0111,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.8
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-3500:DH
 GRAPHICS 2 .8 -3500 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0112,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.7
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-4588:DH
 GRAPHICS 2 .7 -4588 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0113,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.6
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-5239:DH
 GRAPHICS 2 .6 -5239 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0114,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.5
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-5454:DH
 GRAPHICS 2 .5 -5454 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0115,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.4
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-5233:DH
 GRAPHICS 2 .4 -5233 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0116,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.3
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-4575:DH
 GRAPHICS 2 .3 -4575 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0117,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.2
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-3481:DH
 GRAPHICS 2 .2 -3481 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set
 CREATE_NEW_EQUILIBRIUM 0118,1
 CHANGE_STATUS PHASE LIQ=FIX 1
 SET-CONDITION T=1773,P=P0,X(LIQ,B)=.1
 SET_REFERENCE_STATE A LIQ * 1E5
 SET_REFERENCE_STATE B LIQ * 1E5
 EXPERIMENT  HMR(LIQ)=-1950:DH
 GRAPHICS 2 .1 -1950 MS2
 LABEL AH
 SET_ALL_START Y
 Automatic start values will be set

 $
 $ Heat of melting for the compound. T=1341. H(liq)-H(A2B)=3727 J/mol.
 $ This datum has already been used.
 $
 $ Do not forget the following line!
 SAVE_WORKSPACES
PARROT:
PARROT: @@
PARROT: @@ Next file shows how to choose a 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
PARROT: s-o-v 2 0
PARROT: s-o-v 11 0
PARROT: s-o-v 12 0
PARROT: s-o-v 15 0
PARROT: s-o-v 16 0
```

```
PARROT: s-o-v 17 0
PARROT: s-o-v 19 0
PARROT: s-o-v 20 0
PARROT:
PARROT: save
PARROT: @@ Now execute tcex36b.TCM to continue the assessment example
PARROT:Hit RETURN to continue
PARROT: mac tcex36b.TCM
PARROT: s-s-f tcex36
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT: @@ Set alt mode to start
PARROT: s-alt Y
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
15:45:31,684 INFO  Preparing system for use: UNKNOWN_1589204726501
15:45:32,401 INFO  Preparing phase for use: LIQUID
15:45:32,833 INFO  Preparing phase for use: A2B
15:45:33,006 INFO  Preparing phase for use: BCC
   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
15:45:33,161 INFO  Preparing phase for use: FCC
   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
 Changed weight on                      4 equilibria.
ED_EXP: c-a
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: save
ED_EXP: @@ Save changes of weights before leaving the editor
ED_EXP: ba
PARROT: @@ Optimize zero times as a check
PARROT: opt 0
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:45:33



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
```

```
  ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   1.22023362E+03
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   3.21114110E+01

 Number of alternate equilibria                     10

 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   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             3.6380E-12  5.00E+02   4588.       9.176    *
113 HMR(LIQUID)=-5239              0.000      5.00E+02   5239.       10.48    *
114 HMR(LIQUID)=-5454             1.8190E-12  5.00E+02   5454.       10.91    *
115 HMR(LIQUID)=-5233             5.4570E-12  5.00E+02   5233.       10.47    *
116 HMR(LIQUID)=-4575             3.6380E-12  5.00E+02   4575.       9.150    *
117 HMR(LIQUID)=-3481            -3.6380E-12  5.00E+02   3481.       6.962    *
118 HMR(LIQUID)=-1950              0.000      5.00E+02   1950.       3.900


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Note only one error from alternate calculations.
PARROT: @@ This error represents the difference in chemical
PARROT: @@ potentials of the phases.
PARROT: @@ Experiments with just one phase is calculated as normal.
PARROT: @@ Next command supresses the listing of parameters.
```

```
PARROT: s-o-l 1 Y Y N n N
PARROT: l-r C SCREEN


          ==================================================
          OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:45:33



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V2      0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V11     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V12     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V15     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V16     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V17     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V19     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00
 V20     0.00000000E+00    0.00000000E+00    1.00000000E+03    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   1.22023362E+03
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   3.21114110E+01

 Number of alternate equilibria                     10


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                        1.81
   2 Alternate equilibrium calc                                        0.39
2 HTR=3727                        1.5333E+04  5.00E+02  1.1606E+04   23.21    *
   3 Alternate equilibrium calc                                        1.32
   4 Alternate equilibrium calc                                        1.56
   5 Alternate equilibrium calc                                        4.14
   6 Alternate equilibrium calc                                        3.83
  20 Alternate equilibrium calc                                        0.87
  21 Alternate equilibrium calc                                        0.97
  22 Alternate equilibrium calc                                        1.14
  23 Alternate equilibrium calc                                        1.20
100 ACR(B)=0.94                   0.9382      2.89E-02 -1.8474E-03 -6.3948E-02
101 ACR(B)=0.84                   0.8339      2.89E-02 -6.0866E-03 -0.2107
102 ACR(B)=0.74                   0.7297      2.89E-02 -1.0326E-02 -0.3574
103 ACR(B)=0.64                   0.6254      2.89E-02 -1.4565E-02 -0.5042
104 ACR(B)=0.54                   0.5212      2.89E-02 -1.8804E-02 -0.6509
105 ACR(B)=0.44                   0.4170      2.89E-02 -2.3043E-02 -0.7976
106 ACR(B)=0.34                   0.3127      2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23                   0.2085      2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12                   0.1042      2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964              0.000      5.00E+02   1964.       3.928
111 HMR(LIQUID)=-3500             3.6380E-12  5.00E+02   3500.       7.000    *
112 HMR(LIQUID)=-4588             3.6380E-12  5.00E+02   4588.       9.176    *
113 HMR(LIQUID)=-5239              0.000      5.00E+02   5239.       10.48    *
114 HMR(LIQUID)=-5454             1.8190E-12  5.00E+02   5454.       10.91    *
115 HMR(LIQUID)=-5233             5.4570E-12  5.00E+02   5233.       10.47    *
116 HMR(LIQUID)=-4575             3.6380E-12  5.00E+02   4575.       9.150    *
117 HMR(LIQUID)=-3481            -3.6380E-12  5.00E+02   3481.       6.962    *
118 HMR(LIQUID)=-1950              0.000      5.00E+02   1950.       3.900


PARROT:
PARROT: @@ Now optimize
PARROT: opt 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    2 ND ITERATION WE HAVE THE SUM OF SQUARES    1.22026107E+03
  1  1.0000E-04   2  1.0000E-04   3  0.0000E+00   4  0.0000E+00   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.22023821E+03
  1  1.0000E-04   2  0.0000E+00   3  1.0000E-04   4  0.0000E+00   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21985896E+03
  1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  0.0000E+00
  6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00
```

```
     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21985855E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  0.0000E+00   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

     AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21952877E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  1.0000E-04   7  0.0000E+00   8  0.0000E+00   9  0.0000E+00

     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21952862E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  1.0000E-04   7  1.0000E-04   8  0.0000E+00   9  0.0000E+00

     AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21952856E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  1.0000E-04   7  1.0000E-04   8  1.0000E-04   9  0.0000E+00

     AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21945175E+03
 1  1.0000E-04   2  0.0000E+00   3  0.0000E+00   4  1.0000E-04   5  1.0000E-04
 6  1.0000E-04   7  1.0000E-04   8  1.0000E-04   9  1.0000E-04

     AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    1.21347918E+03
 1  1.1575E-04   2 -1.5562E-04   3 -3.9485E-05   4  1.9219E-03   5  1.0209E-04
 6  1.7933E-03   7  1.0073E-04   8  1.0031E-04   9  4.9349E-04

     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.20857820E+03
 1  5.7604E-04   2 -2.8000E-04   3 -5.5554E-04   4  2.9761E-04   5  1.0310E-03
 6  3.2119E-03   7  1.5940E-04   8  5.6558E-04   9  8.6813E-04

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.20419111E+03
 1  1.7516E-03   2 -4.0933E-04   3 -1.8427E-03   4  1.7341E-03   5  1.9072E-03
 6  4.5182E-03   7  3.6464E-04   8 -3.6442E-03   9  1.2034E-03

     AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    1.20018978E+03
 1  4.9648E-03   2 -5.3990E-04   3 -5.3422E-03   4  4.2170E-04   5  1.3347E-03
 6  5.8647E-03   7  1.0916E-03   8 -1.0101E-02   9  1.5910E-03

     AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    1.19656103E+03
 1  8.7053E-03   2 -6.5937E-04   3 -9.4047E-03   4  1.6713E-03   5  2.0974E-03
 6  6.9625E-03   7  1.8270E-03   8 -2.5618E-02   9  1.9085E-03

     AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    1.19290094E+03
 1  1.6702E-02   2 -7.8966E-04   3 -1.8062E-02   4  5.3932E-04   5  2.8046E-03
 6  8.1461E-03   7  3.5323E-03   8 -5.6536E-02   9  2.2985E-03

     AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    1.18895830E+03
 1  2.9858E-02   2 -9.1157E-04   3 -3.2288E-02   4  1.6316E-03   5  6.0823E-03
 6  9.0741E-03   7  6.1592E-03   8 -1.1985E-01   9  2.6324E-03

     AT THE   17 TH ITERATION WE HAVE THE SUM OF SQUARES    1.18371837E+03
 1  5.7117E-02   2 -1.0621E-03   3 -6.1738E-02   4  6.6639E-04   5  1.1595E-02
 6  1.0112E-02   7  1.1749E-02   8 -2.4612E-01   9  3.0842E-03

     AT THE   18 TH ITERATION WE HAVE THE SUM OF SQUARES    1.17576312E+03
 1  1.0981E-01   2 -1.2302E-03   3 -1.1865E-01   4  1.6444E-03   5  2.3333E-02
 6  1.0904E-02   7  2.2419E-02   8 -4.9950E-01   9  3.5580E-03

     AT THE   19 TH ITERATION WE HAVE THE SUM OF SQUARES    1.17580512E+03
 1  1.0990E-01   2 -1.2331E-03   3 -1.1866E-01   4  1.6767E-03   5  2.3329E-02
 6  1.0908E-02   7  2.2420E-02   8 -4.9948E-01   9  3.5631E-03

     AT THE   20 TH ITERATION WE HAVE THE SUM OF SQUARES    1.17576902E+03
 1  1.0981E-01   2 -1.1307E-03   3 -1.1865E-01   4  1.6454E-03   5  2.3333E-02
 6  1.0913E-02   7  2.2419E-02   8 -4.9950E-01   9  3.5581E-03

     AT THE   21 TH ITERATION WE HAVE THE SUM OF SQUARES    1.17573283E+03
 1  1.0983E-01   2 -1.2301E-03   3 -1.1856E-01   4  1.6164E-03   5  2.3336E-02
 6  1.0901E-02   7  2.2419E-02   8 -4.9952E-01   9  3.5536E-03

     AT THE   22 TH ITERATION WE HAVE THE SUM OF SQUARES    1.15839218E+03
 1  2.4518E-01   2 -1.5171E-03   3 -2.6482E-01   4  8.9861E-04   5  8.1369E-02
 6  1.1834E-02   7  4.7658E-02   8 -9.8754E-01   9  4.3315E-03

     AT THE   23 TH ITERATION WE HAVE THE SUM OF SQUARES    1.15852299E+03
 1  2.4519E-01   2 -1.5109E-03   3 -2.6483E-01   4  8.8627E-04   5  8.1438E-02
 6  1.1766E-02   7  4.7658E-02   8 -9.8753E-01   9  4.3220E-03

     AT THE   24 TH ITERATION WE HAVE THE SUM OF SQUARES    1.12429813E+03
 1  5.3084E-01   2 -1.9804E-03   3 -5.7319E-01   4  1.9224E-03   5  3.5638E-01
 6  1.2271E-02   7  9.3910E-02   8 -1.9219E+00   9  5.3987E-03

     AT THE   25 TH ITERATION WE HAVE THE SUM OF SQUARES    1.12430373E+03
 1  5.3084E-01   2 -1.9806E-03   3 -5.7319E-01   4  1.9278E-03   5  3.5639E-01
 6  1.2272E-02   7  9.4010E-02   8 -1.9219E+00   9  5.3997E-03

     AT THE   26 TH ITERATION WE HAVE THE SUM OF SQUARES    1.05801741E+03
 1  1.1108E+00   2 -2.8497E-03   3 -1.1990E+00   4  1.6568E-03   5  1.0413E+00
 6  1.2349E-02   7  1.7987E-01   8 -3.7400E+00   9  7.2585E-03

     AT THE   27 TH ITERATION WE HAVE THE SUM OF SQUARES    1.05799591E+03
 1  1.1108E+00   2 -2.8479E-03   3 -1.1990E+00   4  1.6562E-03   5  1.0413E+00
 6  1.2329E-02   7  1.7987E-01   8 -3.7401E+00   9  7.3562E-03

     AT THE   28 TH ITERATION WE HAVE THE SUM OF SQUARES    9.32316147E+02
 1  2.2754E+00   2 -4.5180E-03   3 -2.4557E+00   4  3.1330E-03   5  2.5155E+00
 6  1.1608E-02   7  3.4709E-01   8 -7.3322E+00   9  1.0723E-02

     AT THE   29 TH ITERATION WE HAVE THE SUM OF SQUARES    9.32175306E+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    9.32266248E+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
```

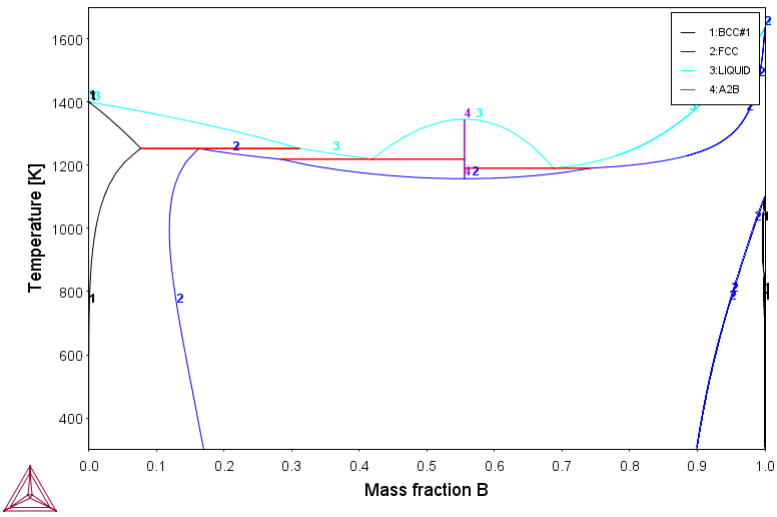
```
 31  2.5901E-03  32  6.6371E-02  33  1.4719E-01  34  2.0341E-01  35  1.9322E-01
 36  7.6393E-02  37  1.5206E-01  38  3.2167E-02  39  3.4860E+00  40  6.2142E+00
 41  8.1446E+00  42  9.2993E+00  43  9.6801E+00  44  9.2873E+00  45  8.1186E+00
 46  6.1762E+00  47  3.4580E+00

                THE SUM OF SQUARES IS   9.32175306E+02
PARROT: cont 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    6.42380269E+02
  1  5.3285E+00   2 -8.7738E-03   3 -5.7408E+00   4  4.7675E-03   5  5.1386E+00
  6  9.8927E-03   7  8.7845E-01   8 -1.4032E+01   9  1.6957E-02

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    3.93290345E+02
  1  8.5797E+00   2 -1.3317E-02   3 -9.2391E+00   4  7.4937E-03   5  8.0040E+00
  6  7.9956E-03   7  1.4404E+00   8 -2.1386E+01   9  2.3783E-02

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    2.09584692E+02
  1  1.1739E+01   2 -1.7636E-02   3 -1.2638E+01   4  9.3817E-03   5  1.0889E+01
  6  5.4398E-03   7  1.9808E+00   8 -2.8820E+01   9  3.0390E-02

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.80934135E+01
  1  1.7814E+01   2 -2.5899E-02   3 -1.9174E+01   4  1.3734E-02   5  1.6703E+01
  6 -6.1020E-06   7  3.0058E+00   8 -4.3892E+01   9  4.3587E-02

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    9.80055082E-01
  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

     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 -1.6297E-03   2 -1.6297E-03   3  1.8276E-04   4  1.5453E-01   5  1.3483E-01
  6 -1.3372E-01   7  5.3418E-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 -3.8162E-04
 26 -3.4080E-01  27 -1.0881E-02  28  7.4579E-02  29 -2.7851E-03  30  2.1226E-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   9.80055082E-01
PARROT: l-r C SCREEN


           ====================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:45:35



 *** OPTIMIZATION ERROR. TOO MANY ITERATIONS ***
     NUMBER OF ITERATIONS:   5


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02691574E+04    0.00000000E+00    1.00000000E+03    1.60588758E+00
 V2     -2.91902485E+01    0.00000000E+00    1.00000000E+03    1.00991504E-02
 V11    -2.18127452E+04    0.00000000E+00    1.00000000E+03    8.65821610E-01
 V12     1.55559538E+01    0.00000000E+00    1.00000000E+03    2.63408130E-03
 V15     1.98563397E+04    0.00000000E+00    1.00000000E+03    1.43532286E+01
 V16    -3.26289208E+00    0.00000000E+00    1.00000000E+03    1.71198633E-02
 V17     3.37569368E+03    0.00000000E+00    1.00000000E+03    4.53503071E+00
 V19    -5.20384289E+04    0.00000000E+00    1.00000000E+03    3.15139854E+01
 V20     5.04396154E+01    0.00000000E+00    1.00000000E+03    2.47933779E-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   9.80055082E-01
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   2.57909232E-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      5.3418E-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  6.0225E-05  2.1226E-03
101 ACR(B)=0.84                  0.8407      2.80E-02  7.1693E-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:Hit RETURN to continue
PARROT: @@ The liquid data fits reasonably. Simplify its parameters.
PARROT: l-p-d liq


 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
PARROT: @@ Rescale the start values of the parameters to current values
PARROT: resc
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02691574E+04    2.02691574E+04    2.02691574E+04    0.00000000E+00
 V2     -2.91902485E+01   -2.91902485E+01   -2.91902485E+01    0.00000000E+00
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     1.98563397E+04    1.98563397E+04    1.98563397E+04    0.00000000E+00
 V16    -3.26289208E+00   -3.26289208E+00   -3.26289208E+00    0.00000000E+00
 V17     3.37569368E+03    3.37569368E+03    3.37569368E+03    0.00000000E+00
 V19    -5.20384289E+04   -5.20384289E+04   -5.20384289E+04    0.00000000E+00
 V20     5.04396154E+01    5.04396154E+01    5.04396154E+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: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y
POLY: 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
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   5 at:   2.413E-01  1.253E+03
 ** LIQUID
    FCC
Calculated.                       6 equilibria

Phase region boundary   6 at:   3.546E-01  1.219E+03
 ** LIQUID
 ** A2B
    FCC

Phase region boundary   7 at:   4.342E-01  1.219E+03
 ** A2B
    FCC
Calculated.                      24 equilibria

Phase region boundary   8 at:   6.572E-01  1.191E+03
 ** LIQUID
 ** A2B
    FCC

Phase region boundary   9 at:   7.154E-01  1.191E+03
 ** LIQUID
    FCC
Calculated                      44 equilibria

Phase region boundary  10 at:   6.257E-01  1.191E+03
 ** LIQUID
    A2B
Calculated.                      23 equilibria
Terminating at known equilibrium

Phase region boundary  11 at:   8.907E-02  3.100E+02
    BCC#1
 ** FCC
Calculated.                      28 equilibria
Terminating at known equilibrium

Phase region boundary  12 at:   8.907E-02  3.100E+02
    BCC#1
 ** FCC
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  13 at:   8.907E-02  3.100E+02
    BCC#1
 ** FCC
Calculated.                      28 equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   4.559E-01  1.196E+03
 ** A2B
    FCC
Calculated.                       3 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   4.559E-01  1.196E+03
 ** A2B
    FCC
Calculated.                      21 equilibria
Terminating at known equilibrium

Phase region boundary  16 at:   6.122E-01  1.168E+03
 ** A2B
    FCC
Calculated.                      16 equilibria
Terminating at known equilibrium
```

```
Phase region boundary  17 at:   6.122E-01  1.168E+03
 ** A2B
    FCC
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   9.533E-01  3.100E+02
    BCC#1
 ** FCC
Calculated..                       2 equilibria
Terminating at axis limit.

Phase region boundary  19 at:   9.530E-01  3.000E+02
    BCC#1
 ** FCC
Calculated                     31 equilibria

Phase region boundary  20 at:   9.533E-01  3.100E+02
    BCC#1
 ** FCC
Calculated                     29 equilibria

Phase region boundary  21 at:   9.533E-01  3.100E+02
    BCC#1
 ** FCC
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   9.533E-01  3.100E+02
    BCC#1
 ** FCC
Calculated                     29 equilibria

Phase region boundary  23 at:   6.769E-02  7.700E+02
    BCC#1
 ** FCC
Calculated..                      15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   6.769E-02  7.700E+02
    BCC#1
 ** FCC
Calculated.                      15 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   9.745E-01  7.700E+02
    BCC#1
 ** FCC
Calculated..                      15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  26 at:   9.745E-01  7.700E+02
    BCC#1
 ** FCC
Calculated                     18 equilibria

Phase region boundary  27 at:   1.086E-01  1.230E+03
    BCC#1
 ** FCC
Calculated..                      28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:   1.086E-01  1.230E+03
    BCC#1
 ** FCC
Calculated.                       2 equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   8.359E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   8.359E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                     37 equilibria

Phase region boundary  31 at:   6.124E-03  1.396E+03
    LIQUID
 ** BCC#1
Calculated                     11 equilibria

Phase region boundary  32 at:   6.124E-03  1.396E+03
    LIQUID
 ** BCC#1
Calculated.                       9 equilibria
Terminating at known equilibrium

Phase region boundary  33 at:   2.658E-01  1.244E+03
    LIQUID
 ** FCC
Calculated.                       2 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   2.658E-01  1.244E+03
    LIQUID
 ** FCC
Calculated.                       5 equilibria
Terminating at known equilibrium

Phase region boundary  35 at:   6.122E-01  1.246E+03
    LIQUID
 ** A2B
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  36 at:   6.122E-01  1.246E+03
    LIQUID
 ** A2B
```

```
 Calculated.                        4 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   9.944E-01  1.601E+03
     LIQUID
  ** FCC
 Calculated.                       33 equilibria
 Terminating at known equilibrium

 Phase region boundary  38 at:   9.944E-01  1.601E+03
     LIQUID
  ** FCC
 Calculated                       12 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     4 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-l d
POST: plot
```




```
POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt 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    9.80055082E-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    9.80047714E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    9.80047684E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    9.79973916E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    9.79973798E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    9.79974048E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    9.80048009E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    9.79974705E-01
  1  1.0001E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    9.74564792E-01
  1  1.0007E+00   2  1.0001E+00   3  1.0074E+00   4  1.0001E+00   5  9.9998E-01
  6  9.9266E-01   7  1.0000E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    9.68319336E-01
  1  1.0001E+00   2  9.9993E-01   3  1.0086E+00   4  1.0048E+00   5  9.9962E-01
  6  9.8903E-01   7  9.9159E-01

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    9.58294052E-01
  1  1.0012E+00   2  9.9951E-01   3  1.0105E+00   4  1.0150E+00   5  9.9882E-01
  6  9.7286E-01   7  9.8384E-01
```

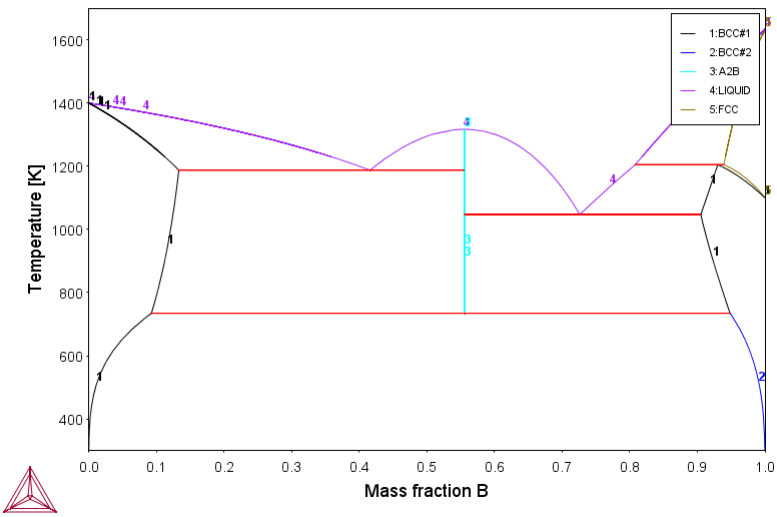
```
     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    9.36471459E-01
  1  9.9970E-01   2  9.9934E-01   3  1.0140E+00   4  1.0400E+00   5  9.9747E-01
  6  9.4967E-01   7  9.6043E-01

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    8.96553883E-01
  1  1.0019E+00   2  9.9883E-01   3  1.0209E+00   4  1.0903E+00   5  9.9477E-01
  6  8.9661E-01   7  9.2172E-01

     AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    8.20178024E-01
  1  9.9941E-01   2  9.9846E-01   3  1.0352E+00   4  1.1942E+00   5  9.8966E-01
  6  7.9747E-01   7  8.3959E-01

     AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    6.87456476E-01
  1  1.0018E+00   2  9.9752E-01   3  1.0636E+00   4  1.4027E+00   5  9.7946E-01
  6  5.9608E-01   7  6.7987E-01

     AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    6.87509881E-01
  1  1.0019E+00   2  9.9752E-01   3  1.0636E+00   4  1.4027E+00   5  9.7946E-01
  6  5.9609E-01   7  6.7985E-01

     AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    6.87455889E-01
  1  1.0018E+00   2  9.9762E-01   3  1.0636E+00   4  1.4027E+00   5  9.7946E-01
  6  5.9608E-01   7  6.7987E-01

     AT THE   17 TH ITERATION WE HAVE THE SUM OF SQUARES    4.93885012E-01
  1  9.9983E-01   2  9.9618E-01   3  1.1210E+00   4  1.8222E+00   5  9.5929E-01
  6  1.9649E-01   7  3.5984E-01

     AT THE   18 TH ITERATION WE HAVE THE SUM OF SQUARES    3.83962944E-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  2.1226E-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   3.83962944E-01
PARROT: resc
PARROT: opt 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    3.83962944E-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    3.83964820E-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    3.83963033E-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    3.83963568E-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    3.83962993E-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    3.83962950E-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    3.83963039E-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    3.83962958E-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  2.1226E-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   3.83962944E-01
PARROT: @@ No change in the parameters, check the diagram again
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
```

```
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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   5 at:   3.781E-01  1.187E+03
  ** LIQUID
  ** A2B
     BCC#1

 Phase region boundary   6 at:   2.888E-01  1.187E+03
  ** LIQUID
     BCC#1
 Calculated                      28 equilibria

 Phase region boundary   7 at:   4.898E-01  1.187E+03
  ** LIQUID
     A2B
 Calculated.                      26 equilibria
```

```
Phase region boundary   8 at:   6.479E-01  1.047E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.629E-01  1.047E+03
    A2B
 ** BCC#1
Calculated.                      10 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.250E-01  1.047E+03
    LIQUID
 ** BCC#1
Calculated.                       9 equilibria

Phase region boundary  11 at:   8.738E-01  1.205E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.791E-01  1.205E+03
    LIQUID
 ** FCC
Calculated                     37 equilibria

Phase region boundary  13 at:   9.347E-01  1.205E+03
    BCC#1
 ** FCC
Calculated                     26 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.657E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                     10 equilibria

Phase region boundary  26 at:   3.657E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                       3 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.657E-01  7.700E+02
 ** A2B
```

```
     BCC#1
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.900E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                      10 equilibria

 Phase region boundary  29 at:   7.900E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                       3 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.900E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                       9 equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.459E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated.                       4 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.459E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated                      26 equilibria

 Phase region boundary  33 at:   8.847E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                       2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.847E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                      29 equilibria

 Phase region boundary  35 at:   6.422E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated                       9 equilibria

 Phase region boundary  36 at:   6.422E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated                      19 equilibria

 Phase region boundary  38 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated.                       4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.219E+03
     LIQUID
  ** A2B
 Calculated.                      12 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.219E+03
     LIQUID
  ** A2B
 Calculated.                       7 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                      20 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      13 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     1 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-l d
POST: plot
```

2020.05.11.15.46.05
A, B
P=1E5, N=1




```
POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Turn off alternate mode and try to calculate all equilibria
PARROT: s-alt Y
 Alternate calculation is on
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a
 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
ED_EXP: s-we 1 alf
 Changed weight on                      4 equilibria.
ED_EXP: s-e 1
 Equilibrium number                      1, label AINV
ED_EXP: c-a
 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
```

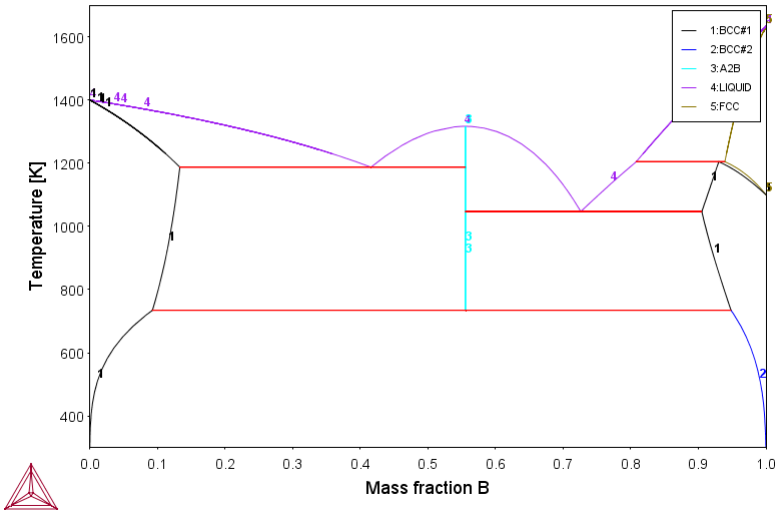
```
 112 AH   < unused >  1773.0      LIQUID
 113 AH   < unused >  1773.0      LIQUID
 114 AH   < unused >  1773.0      LIQUID
 115 AH   < unused >  1773.0      LIQUID
 116 AH   < unused >  1773.0      LIQUID
 117 AH   < unused >  1773.0      LIQUID
 118 AH   < unused >  1773.0      LIQUID
ED_EXP: save
ED_EXP: @@ Save changes
ED_EXP: ba
PARROT: opt 0
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:46:27



 *** 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     -2.90134106E+01   -2.90134106E+01   -2.90134106E+01    3.44753281E-01
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     2.39869521E+04    2.39869521E+04    2.39869521E+04    6.19220671E-01
 V16    -8.02179154E+00   -8.02179154E+00   -8.02179154E+00    2.18789516E+00
 V17     3.13540517E+03    3.13540517E+03    3.13540517E+03    1.44882547E+00
 V19     2.12643608E+04    2.12643608E+04    2.12643608E+04    4.78622190E+00
 V20    -6.23643918E+00   -6.23643918E+00   -6.23643918E+00    1.26468960E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   3.83962944E-01 TO   7.41795979E+00
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   3.37179991E-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 -8.4144E-04
10 W(LIQUID,A)=2E-2              1.9506E-02  2.00E-02 -4.9427E-04 -2.4713E-02
11 W(LIQUID,A)=4.2E-2            4.1827E-02  2.00E-02 -1.7330E-04 -8.6649E-03
12 W(LIQUID,A)=6.5E-2            6.5040E-02  2.00E-02  4.0127E-05  2.0063E-03
13 W(LIQUID,A)=9.3E-2            9.3114E-02  2.00E-02  1.1415E-04  5.7077E-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  1.9748E-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:
PARROT:Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for
PARROT: @@ equilibrium 4. It can be on the wrong side, at high A instead
PARROT: @@  of high B. Try to correct that in the Edit module.
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
 Equilibrium number                      4, label AINV
ED_EXP: s-a-s
T /1204.671472/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /*/: b

 Phase BCC
```

```
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=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
PARROT: @@ The error is still there, calculate the phase diagram.
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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   5 at:   3.781E-01  1.187E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.888E-01  1.187E+03
 ** LIQUID
    BCC#1
Calculated                      28 equilibria

Phase region boundary   7 at:   4.898E-01  1.187E+03
 ** LIQUID
    A2B
Calculated.                      26 equilibria

Phase region boundary   8 at:   6.479E-01  1.047E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.629E-01  1.047E+03
    A2B
 ** BCC#1
Calculated.                      10 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.250E-01  1.047E+03
    LIQUID
 ** BCC#1
Calculated.                       9 equilibria

Phase region boundary  11 at:   8.738E-01  1.205E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.791E-01  1.205E+03
    LIQUID
 ** FCC
Calculated                      37 equilibria

Phase region boundary  13 at:   9.347E-01  1.205E+03
    BCC#1
 ** FCC
Calculated                      26 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      14 equilibria
```

```
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.657E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                      10 equilibria

Phase region boundary  26 at:   3.657E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.657E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.900E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                      10 equilibria

Phase region boundary  29 at:   7.900E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.900E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.459E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.459E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated                      26 equilibria

Phase region boundary  33 at:   8.847E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.847E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                      29 equilibria

Phase region boundary  35 at:   6.422E-03  1.397E+03
    LIQUID
 ** BCC#1
Calculated                      9 equilibria

Phase region boundary  36 at:   6.422E-03  1.397E+03
    LIQUID
 ** BCC#1
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.299E-01  1.244E+03
    LIQUID
 ** BCC#1
Calculated                      19 equilibria

Phase region boundary  38 at:   2.299E-01  1.244E+03
    LIQUID
 ** BCC#1
```

```
 Calculated.                      4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.219E+03
     LIQUID
  ** A2B
 Calculated.                     12 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.219E+03
     LIQUID
  ** A2B
 Calculated.                      7 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                     20 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                     13 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                      1 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-l d
POST: plot
   2020.05.11.15.46.33
   A, B
   P=1E5, N=1
```




```
POST:
POST: set-inter
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
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: ed
ED_EXP: read 1
ED_EXP: s-we 0 4
ED_EXP: save
ED_EXP: ba
PARROT: opt 0
 Use      25 experiments, maximum is        2000
 Use     494 real workspace, maximum is    50000
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:46:55



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==
```

```
 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02757864E+04    2.02757864E+04    2.02757864E+04    7.39333291E-02
 V2     -2.90134106E+01   -2.90134106E+01   -2.90134106E+01    3.44753281E-01
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     2.39869521E+04    2.39869521E+04    2.39869521E+04    6.19220671E-01
 V16    -8.02179154E+00   -8.02179154E+00   -8.02179154E+00    2.18789516E+00
 V17     3.13540517E+03    3.13540517E+03    3.13540517E+03    1.44882547E+00
 V19     2.12643608E+04    2.12643608E+04    2.12643608E+04    4.78622190E+00
 V20    -6.23643918E+00   -6.23643918E+00   -6.23643918E+00    1.26468960E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   3.83962944E-01 TO   7.37821203E+00
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   4.09900669E-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 -8.4144E-04
10 W(LIQUID,A)=2E-2              1.9506E-02  2.00E-02 -4.9427E-04 -2.4713E-02
11 W(LIQUID,A)=4.2E-2            4.1827E-02  2.00E-02 -1.7330E-04 -8.6649E-03
12 W(LIQUID,A)=6.5E-2            6.5040E-02  2.00E-02  4.0127E-05  2.0063E-03
13 W(LIQUID,A)=9.3E-2            9.3114E-02  2.00E-02  1.1415E-04  5.7077E-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  1.9748E-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:
PARROT:Hit RETURN to continue
PARROT: opt 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    7.37821203E+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    7.53023017E+00
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    7.11521779E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    7.10972309E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    7.11102690E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    7.10986731E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    7.10934830E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    7.10948638E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    3.63975208E-01
  1  9.9778E-01   2  1.0040E+00   3  1.0002E+00   4  9.9998E-01   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    3.27817554E-01
  1  9.9774E-01   2  1.0037E+00   3  1.0002E+00   4  9.9757E-01   5  9.9826E-01
  6  1.0015E+00   7  1.0030E+00

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    2.68439488E-01
  1  9.9735E-01   2  1.0038E+00   3  9.9865E-01   4  9.9067E-01   5  9.9310E-01
  6  1.0027E+00   7  1.0046E+00

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    2.16951991E-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    1.51362471E-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
```

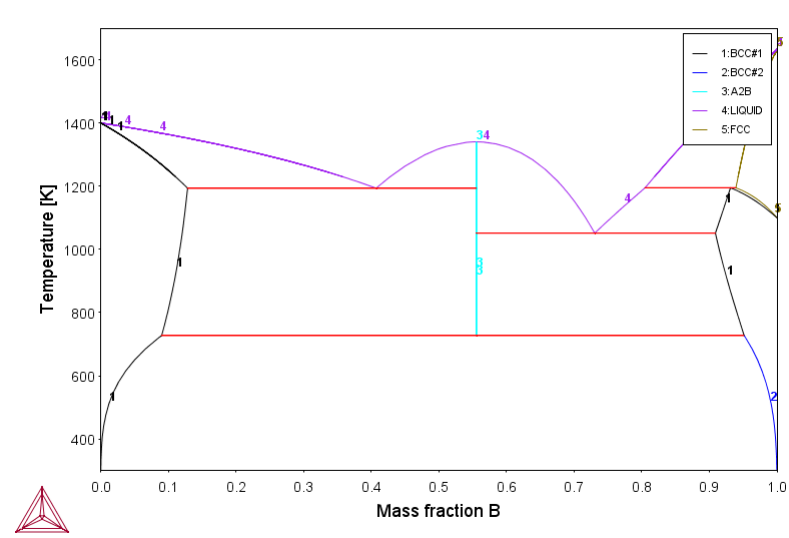
```
  1  7.0456E-02   2 -3.9714E-02   3 -7.7916E-02   4 -7.3555E-02   5  5.9816E-02
  6  2.5625E-01   7 -1.8710E-02   8 -9.5446E-02   9  1.6592E-01  10  5.4874E-02
 11 -3.7948E-02  12  3.1686E-02  13 -9.3444E-02  14 -2.8662E-02  15 -1.6941E-02
 16 -1.0568E-02  17 -1.1806E-02  18 -1.9276E-03  19 -9.4029E-03  20  5.1591E-02
 21 -1.0494E-02  22  4.5737E-02  23  2.4191E-03  24  1.2336E-02  25 -8.0307E-02

               THE SUM OF SQUARES IS   1.51362471E-01
PARROT: cont 30

 It is safe to CONTINUE only after TOO MANY ITERATIONS
 and no change in variables and experiments ...
 Now anything can happen ...

PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:46:55



 *** 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      2.01874454E+04    2.02757864E+04    2.02757864E+04    2.69317709E-02
 V2     -2.90969456E+01   -2.90134106E+01   -2.90134106E+01    1.50773051E-02
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     2.37258689E+04    2.39869521E+04    2.39869521E+04    9.90009419E-02
 V16    -7.64417352E+00   -8.02179154E+00   -8.02179154E+00    3.01534400E-01
 V17     3.02274856E+03    3.13540517E+03    3.13540517E+03    2.49736584E-01
 V19     2.14534092E+04    2.12643608E+04    2.12643608E+04    6.60455769E-01
 V20    -6.31332836E+00   -6.23643918E+00   -6.23643918E+00    1.71543865E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   7.37821203E+00 TO   1.51362471E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.40902619E-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.       2.563      0.2563
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  5.4874E-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 -5.7325E-04 -2.8662E-02
11 W(LIQUID,A)=4.2E-2          4.1661E-02  2.00E-02 -3.3883E-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 -3.8552E-05 -1.9276E-03
20 W(FCC,A)=3.8E-2             3.7812E-02  2.00E-02 -1.8806E-04 -9.4029E-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  9.1475E-04  4.5737E-02
22 W(FCC,A)=5.9E-2             5.9048E-02  2.00E-02  4.8381E-05  2.4191E-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:Hit RETURN to continue
PARROT: @@ Optimization converged, try to add equilibrium 4 again
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
 Equilibrium number                     4, label AINV
ED_EXP: s-a-s
T /1204.671472/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
```

```
ED_EXP: c-e
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=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
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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   5 at:   3.764E-01  1.194E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.817E-01  1.194E+03
 ** LIQUID
    BCC#1
Calculated                      25 equilibria

Phase region boundary   7 at:   4.860E-01  1.194E+03
 ** LIQUID
    A2B
Calculated.                      28 equilibria

Phase region boundary   8 at:   6.504E-01  1.052E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.656E-01  1.052E+03
    A2B
 ** BCC#1
Calculated.                      11 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.290E-01  1.052E+03
    LIQUID
 ** BCC#1
Calculated.                       8 equilibria

Phase region boundary  11 at:   8.731E-01  1.195E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.778E-01  1.195E+03
    LIQUID
 ** FCC
Calculated                      31 equilibria

Phase region boundary  13 at:   9.353E-01  1.195E+03
    BCC#1
 ** FCC
Calculated                      21 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
```

```
 ** BCC#2
Calculated..                        2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                        13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                        2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                        13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                        2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                        13 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.649E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                        10 equilibria

Phase region boundary  26 at:   3.649E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                         3 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.649E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                        14 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.918E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                        10 equilibria

Phase region boundary  29 at:   7.918E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                         3 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.918E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                        10 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.447E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated.                         4 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.447E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated                        26 equilibria

Phase region boundary  33 at:   8.855E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                         3 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.855E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                        29 equilibria

Phase region boundary  35 at:   6.403E-03  1.397E+03
    LIQUID
 ** BCC#1
Calculated                         9 equilibria

Phase region boundary  36 at:   6.403E-03  1.397E+03
    LIQUID
 ** BCC#1
Calculated.                        13 equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.294E-01  1.244E+03
    LIQUID
 ** BCC#1
Calculated                        21 equilibria

Phase region boundary  38 at:   2.294E-01  1.244E+03
    LIQUID
 ** BCC#1
Calculated.                         4 equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.242E+03
```

```
     LIQUID
  ** A2B
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.242E+03
     LIQUID
  ** A2B
 Calculated.                       8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                      20 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      13 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     0 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-l d
POST: plot
```




```
POST:
POST: set-inter
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
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-r C SCREEN


            ====================================================
            OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:47:35



 *** 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      2.01874454E+04    2.02757864E+04    2.02757864E+04    2.69317709E-02
 V2     -2.90969456E+01   -2.90134106E+01   -2.90134106E+01    1.50773051E-02
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     2.37258689E+04    2.39869521E+04    2.39869521E+04    9.90009419E-02
 V16    -7.64417352E+00   -8.02179154E+00   -8.02179154E+00    3.01534400E-01
 V17     3.02274856E+03    3.13540517E+03    3.13540517E+03    2.49736584E-01
 V19     2.14534092E+04    2.12643608E+04    2.12643608E+04    6.60455769E-01
 V20    -6.31332836E+00   -6.23643918E+00   -6.23643918E+00    1.71543865E+00
```

```
 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   7.37821203E+00 TO   1.51362471E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.40902619E-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.       2.563      0.2563
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  5.4874E-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 -5.7325E-04 -2.8662E-02
11 W(LIQUID,A)=4.2E-2            4.1661E-02  2.00E-02 -3.3883E-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 -3.8552E-05 -1.9276E-03
20 W(FCC,A)=3.8E-2               3.7812E-02  2.00E-02 -1.8806E-04 -9.4029E-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  9.1475E-04  4.5737E-02
22 W(FCC,A)=5.9E-2               5.9048E-02  2.00E-02  4.8381E-05  2.4191E-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
PARROT: opt 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    1.51362471E-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    1.52527852E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    1.53435326E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.50566185E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50808966E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50605638E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50498134E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50519401E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50296937E-01
  1  9.9999E-01   2  1.0000E+00   3  1.0001E+00   4  9.9998E-01   5  9.9999E-01
  6  1.0001E+00   7  1.0001E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50105758E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  9.9996E-01   5  9.9998E-01
  6  1.0002E+00   7  1.0002E+00

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49912038E-01
  1  9.9999E-01   2  1.0000E+00   3  1.0002E+00   4  9.9992E-01   5  9.9996E-01
  6  1.0002E+00   7  1.0003E+00

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49696733E-01
  1  9.9999E-01   2  1.0000E+00   3  1.0002E+00   4  9.9986E-01   5  9.9992E-01
  6  1.0004E+00   7  1.0007E+00

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49438056E-01
  1  9.9998E-01   2  1.0000E+00   3  1.0002E+00   4  9.9974E-01   5  9.9985E-01
  6  1.0007E+00   7  1.0014E+00

      AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49082954E-01
  1  9.9998E-01   2  1.0000E+00   3  1.0001E+00   4  9.9950E-01   5  9.9971E-01
  6  1.0013E+00   7  1.0029E+00

      AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48546278E-01
  1  9.9996E-01   2  1.0000E+00   3  1.0000E+00   4  9.9904E-01   5  9.9942E-01
  6  1.0024E+00   7  1.0058E+00

      AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    1.49187671E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  9.9904E-01   5  9.9942E-01
  6  1.0025E+00   7  1.0058E+00

      AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50820323E-01
  1  9.9998E-01   2  1.0001E+00   3  1.0000E+00   4  9.9903E-01   5  9.9942E-01
```

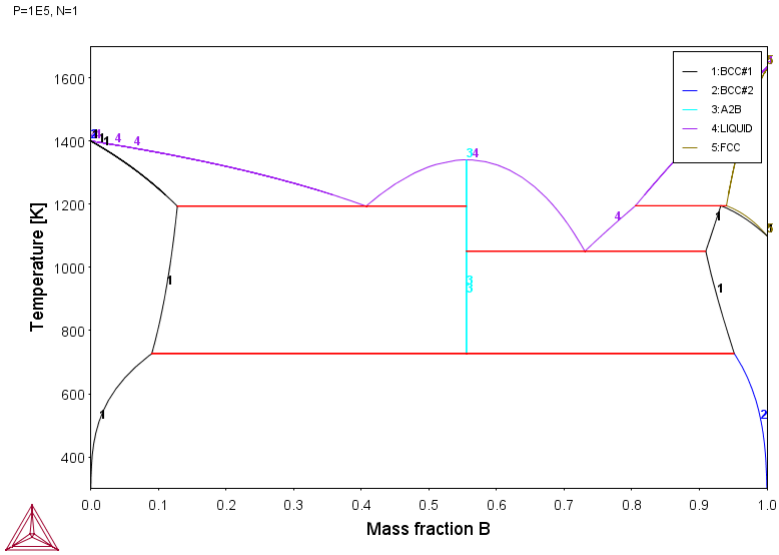
```
  6  1.0024E+00   7  1.0058E+00

      AT THE   17 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48143914E-01
  1  9.9998E-01   2  9.9998E-01   3  1.0001E+00   4  9.9903E-01   5  9.9942E-01
  6  1.0024E+00   7  1.0058E+00

      AT THE   18 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48101120E-01
  1  9.9997E-01   2  1.0000E+00   3  1.0001E+00   4  9.9912E-01   5  9.9942E-01
  6  1.0024E+00   7  1.0059E+00

      AT THE   19 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48098570E-01
  1  9.9996E-01   2  1.0000E+00   3  1.0001E+00   4  9.9911E-01   5  9.9951E-01
  6  1.0025E+00   7  1.0059E+00

      AT THE   20 TH ITERATION WE HAVE THE SUM OF SQUARES    1.47343756E-01
  1  9.9995E-01   2  9.9998E-01   3  9.9990E-01   4  9.9819E-01   5  9.9893E-01
  6  1.0048E+00   7  1.0117E+00

      AT THE   21 TH ITERATION WE HAVE THE SUM OF SQUARES    1.48037496E-01
  1  9.9997E-01   2  9.9996E-01   3  9.9986E-01   4  9.9823E-01   5  9.9895E-01
  6  1.0047E+00   7  1.0117E+00

      AT THE   22 TH ITERATION WE HAVE THE SUM OF SQUARES    1.46170283E-01
  1  9.9990E-01   2  9.9997E-01   3  9.9943E-01   4  9.9635E-01   5  9.9778E-01
  6  1.0094E+00   7  1.0234E+00

      AT THE   23 TH ITERATION WE HAVE THE SUM OF SQUARES    1.44754656E-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    1.44422276E-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 -7.7951E-03
 16 -8.4318E-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   1.44422276E-01
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:47:35



 *** 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      2.01820940E+04    2.01874454E+04    2.01874454E+04    2.60519732E-02
 V2     -2.90936148E+01   -2.90969456E+01   -2.90969456E+01    1.41576512E-02
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     2.36701118E+04    2.37258689E+04    2.37258689E+04    1.00528934E-01
 V16    -7.56541436E+00   -7.64417352E+00   -7.64417352E+00    3.17218673E-01
 V17     3.00342376E+03    3.02274856E+03    3.02274856E+03    2.60675577E-01
 V19     2.20133191E+04    2.14534092E+04    2.14534092E+04    6.92924706E-01
 V20    -6.72498142E+00   -6.31332836E+00   -6.31332836E+00    1.79242859E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.51362471E-01 TO   1.44422276E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.02345979E-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.      0.6681      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 -2.1691E-03 -0.1085
10 W(LIQUID,A)=2E-2              1.9541E-02  2.00E-02 -4.5856E-04 -2.2928E-02
11 W(LIQUID,A)=4.2E-2            4.1844E-02  2.00E-02 -1.5590E-04 -7.7951E-03
12 W(LIQUID,A)=6.5E-2            6.4983E-02  2.00E-02 -1.6864E-05 -8.4318E-04
13 W(LIQUID,A)=9.3E-2            9.2906E-02  2.00E-02 -9.3700E-05 -4.6850E-03
```

```
20 W(LIQUID,A)=0.104             0.1041      2.00E-02  6.5961E-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 -2.7609E-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: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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   5 at:   3.763E-01  1.194E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.815E-01  1.194E+03
 ** LIQUID
    BCC#1
Calculated                      27 equilibria

Phase region boundary   7 at:   4.860E-01  1.194E+03
 ** LIQUID
    A2B
Calculated.                      28 equilibria

Phase region boundary   8 at:   6.505E-01  1.051E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.660E-01  1.051E+03
    A2B
 ** BCC#1
Calculated.                      11 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.294E-01  1.051E+03
    LIQUID
 ** BCC#1
Calculated.                       8 equilibria

Phase region boundary  11 at:   8.737E-01  1.195E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.785E-01  1.195E+03
    LIQUID
 ** FCC
Calculated                      30 equilibria

Phase region boundary  13 at:   9.360E-01  1.195E+03
    BCC#1
 ** FCC
Calculated                      28 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
```

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

 Phase region boundary  24 at:   7.140E-01  3.100E+02
  ** BCC#1
     BCC#2
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   3.650E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                      10 equilibria

 Phase region boundary  26 at:   3.650E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                       3 equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   3.650E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                      14 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.919E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                      10 equilibria

 Phase region boundary  29 at:   7.919E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                       3 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.919E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                      10 equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.445E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated.                       4 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.445E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated                      26 equilibria

 Phase region boundary  33 at:   8.860E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                       2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.860E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                      29 equilibria

 Phase region boundary  35 at:   6.399E-03  1.397E+03
     LIQUID
  ** BCC#2
 Calculated                      10 equilibria

 Phase region boundary  36 at:   6.399E-03  1.397E+03
     LIQUID
  ** BCC#2
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.293E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated                      21 equilibria

 Phase region boundary  38 at:   2.293E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated.                       4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.242E+03
     LIQUID
  ** A2B
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.242E+03
     LIQUID
  ** A2B
 Calculated.                       8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                      20 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      12 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     1 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes
```

```
POST: s-l d
POST: plot
```




```
POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid
PARROT: @@ at high B. Restore equilibrium 4 on the POP file
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
 Equilibrium number                     4, label AINV
ED_EXP: s-we 1
Equilibria (range) or label(s) /PRESENT/: PRESENT
ED_EXP: s-a-s
T /1204.671472/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
 Testing result with global minimization
    14 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=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
ED_EXP: ba
PARROT: resc
PARROT: opt 0
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r C SCREEN


            ==================================================
            OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:48: 2
```

```
 *** 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      2.01820940E+04    2.01820940E+04    2.01820940E+04    0.00000000E+00
 V2     -2.90936148E+01   -2.90936148E+01   -2.90936148E+01    0.00000000E+00
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     2.36701118E+04    2.36701118E+04    2.36701118E+04    0.00000000E+00
 V16    -7.56541436E+00   -7.56541436E+00   -7.56541436E+00    0.00000000E+00
 V17     3.00342376E+03    3.00342376E+03    3.00342376E+03    0.00000000E+00
 V19     2.20133191E+04    2.20133191E+04    2.20133191E+04    0.00000000E+00
 V20    -6.72498142E+00   -6.72498142E+00   -6.72498142E+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   8.21385634E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   3.73357106E-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.      0.6681      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 -2.1691E-03 -0.1085
10 W(LIQUID,A)=2E-2              1.9541E-02  2.00E-02 -4.5856E-04 -2.2928E-02
11 W(LIQUID,A)=4.2E-2            4.1844E-02  2.00E-02 -1.5590E-04 -7.7951E-03
12 W(LIQUID,A)=6.5E-2            6.4983E-02  2.00E-02 -1.6864E-05 -8.4318E-04
13 W(LIQUID,A)=9.3E-2            9.2906E-02  2.00E-02 -9.3700E-05 -4.6850E-03
20 W(LIQUID,A)=0.104             0.1041      2.00E-02  6.5961E-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 -2.7609E-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
 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    8.21385634E-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    8.22203961E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    8.23998052E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    8.41432007E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    8.13827121E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    8.12101224E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    7.96528711E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0000E+00
```

```
     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    8.02190128E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0001E+00

     AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    2.23897027E-01
  1  1.0000E+00   2  1.0000E+00   3  9.9684E-01   4  1.0013E+00   5  1.0004E+00
  6  1.0026E+00   7  9.9908E-01

     AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    2.14210742E-01
  1  1.0000E+00   2  9.9989E-01   3  9.9763E-01   4  1.0026E+00   5  1.0012E+00
  6  1.0043E+00   7  1.0027E+00

     AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    2.02681760E-01
  1  1.0001E+00   2  1.0000E+00   3  9.9857E-01   4  1.0047E+00   5  1.0024E+00
  6  1.0073E+00   7  1.0104E+00

     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.86048556E-01
  1  1.0003E+00   2  1.0001E+00   3  1.0009E+00   4  1.0098E+00   5  1.0054E+00
  6  1.0128E+00   7  1.0246E+00

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.70124823E-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    1.67849058E-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 -6.8334E-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  4.0014E-04  20  7.0613E-03
 21 -6.1541E-04  22  4.9461E-03  23 -1.7571E-03  24  4.0977E-02  25 -2.3417E-02
 26 -2.5371E-03  27 -6.9023E-02  28  2.0311E-02  29 -7.1933E-02

              THE SUM OF SQUARES IS   1.67849058E-01
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:48: 2



 *** 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      2.02022872E+04    2.01820940E+04    2.01820940E+04    2.48851192E-02
 V2     -2.91083466E+01   -2.90936148E+01   -2.90936148E+01    1.36092983E-02
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     2.38442460E+04    2.36701118E+04    2.36701118E+04    8.28181316E-02
 V16    -7.75413088E+00   -7.56541436E+00   -7.56541436E+00    2.55327586E-01
 V17     3.04598874E+03    3.00342376E+03    3.00342376E+03    2.36433693E-01
 V19     2.26500728E+04    2.20133191E+04    2.20133191E+04    4.73555874E-01
 V20    -7.18046403E+00   -6.72498142E+00   -6.72498142E+00    1.24878465E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.21385634E-01 TO   1.67849058E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   7.62950265E-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     -6.8334E-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  8.0027E-06  4.0014E-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 -1.2308E-05 -6.1541E-04
20 W(LIQUID,A)=0.104             0.1041      2.00E-02  9.8921E-05  4.9461E-03
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20 W(FCC,A)=3.8E-2                3.7965E-02  2.00E-02 -3.5141E-05 -1.7571E-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 -5.0741E-05 -2.5371E-03
22 W(FCC,A)=5.9E-2                5.7620E-02  2.00E-02 -1.3805E-03 -6.9023E-02
23 W(LIQUID,A)=0.245              0.2454      2.00E-02  4.0622E-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:
PARROT:Hit RETURN to continue
PARROT: @@ Now optimize all parameters and all experiments
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02022872E+04    2.01820940E+04    2.01820940E+04    2.48851192E-02
 V2     -2.91083466E+01   -2.90936148E+01   -2.90936148E+01    1.36092983E-02
 V11    -2.18127452E+04
 V12     1.55559538E+01
 V15     2.38442460E+04    2.36701118E+04    2.36701118E+04    8.28181316E-02
 V16    -7.75413088E+00   -7.56541436E+00   -7.56541436E+00    2.55327586E-01
 V17     3.04598874E+03    3.00342376E+03    3.00342376E+03    2.36433693E-01
 V19     2.26500728E+04    2.20133191E+04    2.20133191E+04    4.73555874E-01
 V20    -7.18046403E+00   -6.72498142E+00   -6.72498142E+00    1.24878465E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.21385634E-01 TO   1.67849058E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   7.62950265E-03
PARROT: s-o-v 11-12
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a
 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
ED_EXP: s-e 1
 Equilibrium number                      1, label AINV
ED_EXP: c-a
 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
ED_EXP: ba
PARROT: opt 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    5.15868594E-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    5.16672890E-01
 1  1.0011E+00   2  1.0005E+00   3  1.0000E+00   4  1.0000E+00   5  1.0074E+00
 6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

     AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    5.18517323E-01
 1  1.0010E+00   2  1.0006E+00   3  1.0000E+00   4  1.0000E+00   5  1.0074E+00
 6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

     AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    5.10048069E-01
 1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
 6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

     AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    5.14678829E-01
 1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0001E+00   5  1.0074E+00
 6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10329453E-01
 1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0075E+00
 6  1.0249E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

     AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10036853E-01
 1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
 6  1.0250E+00   7  1.0142E+00   8  1.0289E+00   9  1.0677E+00

     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10043894E-01
 1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
 6  1.0250E+00   7  1.0143E+00   8  1.0289E+00   9  1.0677E+00

     AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10201104E-01
 1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
 6  1.0250E+00   7  1.0142E+00   8  1.0290E+00   9  1.0677E+00

     AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    5.10021788E-01
 1  1.0010E+00   2  1.0005E+00   3  1.0001E+00   4  1.0000E+00   5  1.0074E+00
 6  1.0250E+00   7  1.0142E+00   8  1.0289E+00   9  1.0678E+00

     AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    4.31523143E-01
 1  1.0007E+00   2  1.0011E+00   3  1.0017E+00   4  9.9872E-01   5  1.0073E+00
 6  1.0250E+00   7  1.0142E+00   8  1.0289E+00   9  1.0678E+00

     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    3.87996639E-01
 1  1.0007E+00   2  1.0016E+00   3  1.0015E+00   4  9.9831E-01   5  1.0076E+00
 6  1.0269E+00   7  1.0145E+00   8  1.0283E+00   9  1.0674E+00

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    3.46562259E-01
 1  1.0012E+00   2  1.0021E+00   3  1.0017E+00   4  9.9707E-01   5  1.0078E+00
 6  1.0307E+00   7  1.0152E+00   8  1.0271E+00   9  1.0665E+00

     AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    2.88306751E-01
 1  1.0019E+00   2  1.0031E+00   3  1.0011E+00   4  9.9524E-01   5  1.0092E+00
 6  1.0382E+00   7  1.0164E+00   8  1.0246E+00   9  1.0647E+00

     AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    2.01084743E-01
 1  1.0035E+00   2  1.0050E+00   3  1.0003E+00   4  9.9135E-01   5  1.0119E+00
 6  1.0533E+00   7  1.0190E+00   8  1.0194E+00   9  1.0612E+00

     AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    9.39280682E-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    6.73924415E-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  1.3392E-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   6.73924415E-02
PARROT: l-r C SCREEN


          ==================================================
          OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:48: 3



 *** 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
```

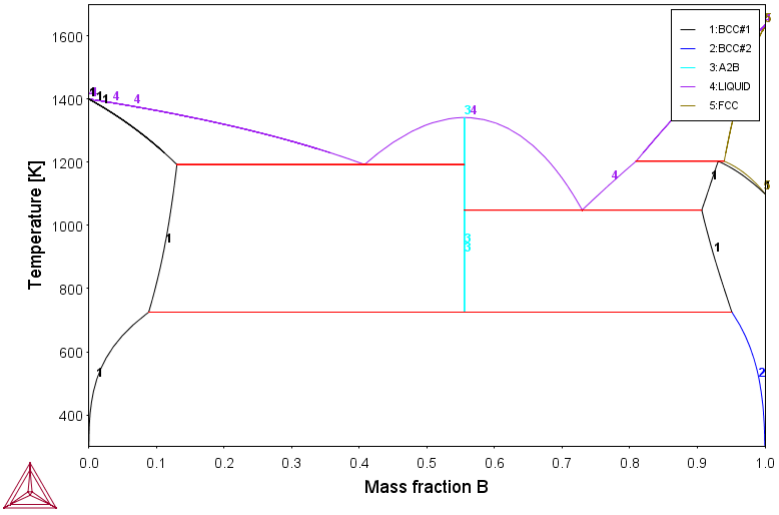
```
 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820940E+04    2.01820940E+04    3.02498609E-02
 V2     -2.94290453E+01   -2.90936148E+01   -2.90936148E+01    2.30117886E-02
 V11    -2.17328114E+04   -2.18127452E+04   -2.18127452E+04    3.47139480E-02
 V12     1.52102756E+01    1.55559538E+01    1.55559538E+01    5.38555607E-02
 V15     2.42012671E+04    2.36701118E+04    2.36701118E+04    8.60925907E-02
 V16    -8.38545766E+00   -7.56541436E+00   -7.56541436E+00    2.83695257E-01
 V17     3.08774212E+03    3.00342376E+03    3.00342376E+03    2.37803061E-01
 V19     2.20600544E+04    2.20133191E+04    2.20133191E+04    4.87694939E-01
 V20    -7.07096147E+00   -6.72498142E+00   -6.72498142E+00    1.27666146E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15868594E-01 TO   6.73924415E-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  1.3392E-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 -2.9644E-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:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram one last time.
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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   5 at:   3.771E-01  1.192E+03
  ** LIQUID
  ** A2B
     BCC#1

 Phase region boundary   6 at:   2.828E-01  1.192E+03
  ** LIQUID
     BCC#1
 Calculated                      28 equilibria

 Phase region boundary   7 at:   4.863E-01  1.192E+03
  ** LIQUID
     A2B
 Calculated.                      28 equilibria

 Phase region boundary   8 at:   6.500E-01  1.048E+03
  ** LIQUID
     A2B
  ** BCC#1

 Phase region boundary   9 at:   7.639E-01  1.048E+03
     A2B
  ** BCC#1
 Calculated.                      11 equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   8.273E-01  1.048E+03
     LIQUID
  ** BCC#1
 Calculated.                       8 equilibria

 Phase region boundary  11 at:   8.748E-01  1.203E+03
     LIQUID
  ** BCC#1
  ** FCC

 Phase region boundary  12 at:   8.799E-01  1.203E+03
     LIQUID
  ** FCC
 Calculated                      35 equilibria

 Phase region boundary  13 at:   9.353E-01  1.203E+03
     BCC#1
  ** FCC
```

```
Calculated                     24 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.647E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                     10 equilibria

Phase region boundary  26 at:   3.647E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.647E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                     14 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.910E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                     10 equilibria

Phase region boundary  29 at:   7.910E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.910E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.448E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.448E-01  1.230E+03
 ** LIQUID
    BCC#1
```

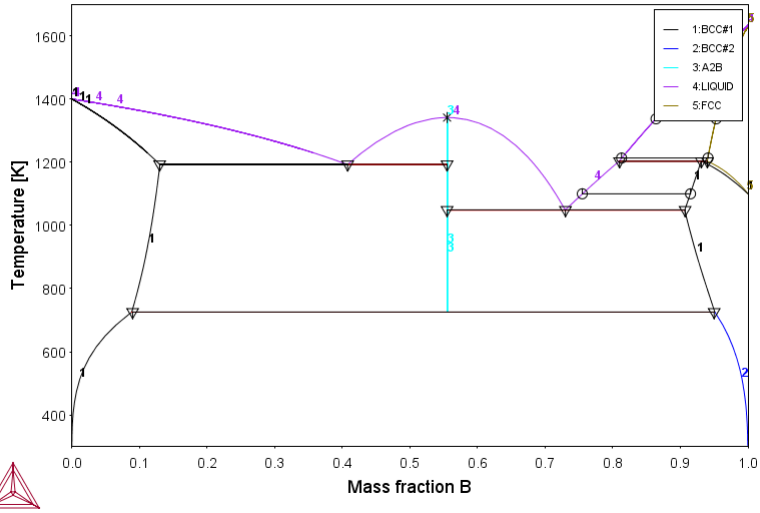
```
 Calculated                      26 equilibria

 Phase region boundary  33 at:   8.858E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                      2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.858E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                      29 equilibria

 Phase region boundary  35 at:   6.415E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated                      13 equilibria

 Phase region boundary  36 at:   6.415E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated.                     13 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated                      23 equilibria

 Phase region boundary  38 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated.                      4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated.                     14 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated.                      8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                     20 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      9 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                      1 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-l d
POST: plot
```

2020.05.11.15.48.07
A, B
P=1E5, N=1



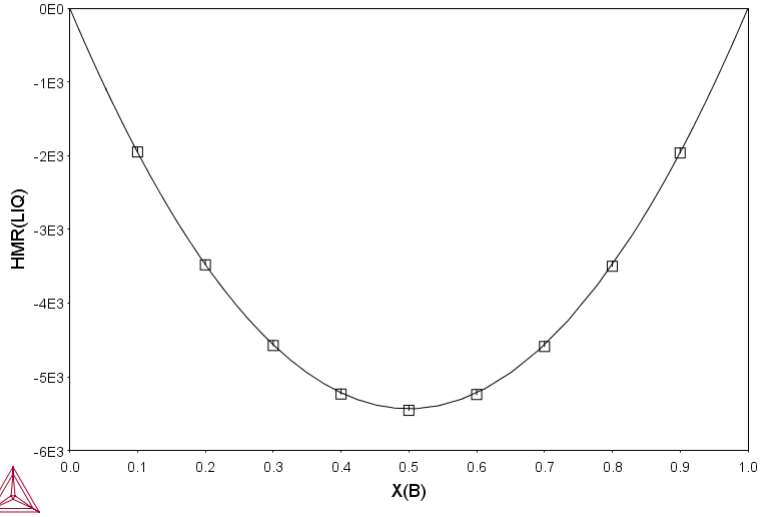

```
POST:
POST: set-inter
POST:Hit RETURN to continue
POST: @@ Add the experimental data
POST: a-e-d y exp36 0; 1
POST: plot
```

2020.05.11.15.48.30
A, B
P=1E5, N=1




```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
POLY: read,,,
POLY:
POLY:
POLY: s-a-v 2 none
POLY: s-c t=1773
POLY: c-e
 Using global minimization procedure
Calculated           628 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: sh hmr
 HMR=13116.476
POLY: l-st c
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 A                        ENTERED   SER
 B                        ENTERED   SER
POLY: s-r-s a liq * 1e5
POLY: s-r-s b liq * 1e5
POLY: save tcex36h y
POLY: step normal
 No initial equilibrium, using default
 Step will start from axis value   0.123400
...OK

 Phase Region from   0.123400     for:
     LIQUID
 Global test at  3.23400E-01 .... OK
 Global test at  5.73400E-01 .... OK
 Global test at  8.23400E-01 .... OK
 Global test at  9.53400E-01 .... OK
 Global test at  1.00000E+00 .... OK
 Terminating at    1.00000
 Calculated    51 equilibria

 Phase Region from   0.123400     for:
     LIQUID
 Global test at  8.34000E-02 .... OK
 Global test at  3.34000E-02 .... OK
 Terminating at   0.250000E-11
 Calculated    28 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36h.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x x(b)
POST: s-d-a y hmr(liq)
POST: a-e-d y exp36 0; 2
POST: plot
```

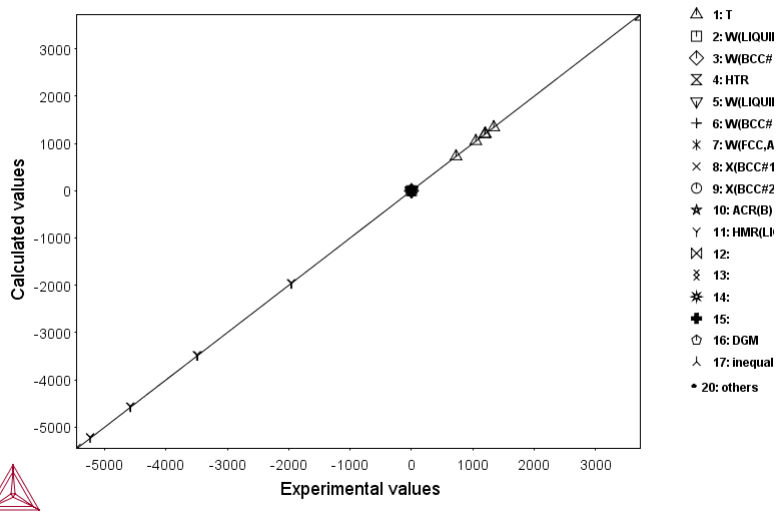
2020.05.11.15.48.52
A, B
T=1773, P=1E5, N=1



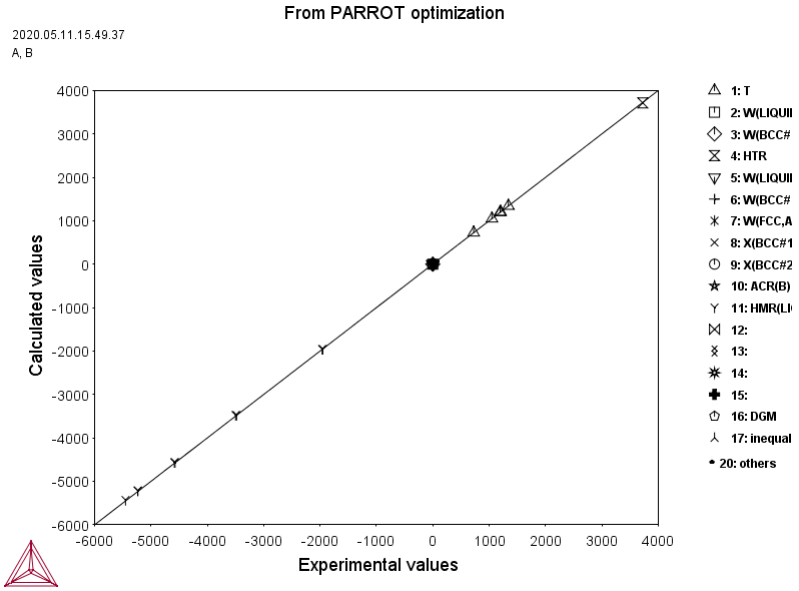

```
POST:
POST:Hit RETURN to continue
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-result gra pexp36 1,
```

From PARROT optimization

2020.05.11.15.49.15
A, B




```
POST: s-s-s y n -6000 4000
POST: s-s-s x n -6000 4000
POST: plot
```




```
POST: b
PARROT: set-inter
PARROT: set-inter
PARROT:
```

tcex36a-tcex36b

```
PARROT:About
 NO SUCH COMMAND, USE HELP
PARROT:PARROT:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36b.TCM.test"
PARROT: s-s-f tcex36
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820940E+04    2.01820940E+04    3.02498609E-02
 V2     -2.94290453E+01   -2.90936148E+01   -2.90936148E+01    2.30117886E-02
 V11    -2.17328114E+04   -2.18127452E+04   -2.18127452E+04    3.47139480E-02
 V12     1.52102756E+01    1.55559538E+01    1.55559538E+01    5.38555607E-02
 V15     2.42012671E+04    2.36701118E+04    2.36701118E+04    8.60925907E-02
 V16    -8.38545766E+00   -7.56541436E+00   -7.56541436E+00    2.83695257E-01
 V17     3.08774212E+03    3.00342376E+03    3.00342376E+03    2.37803061E-01
 V19     2.20600544E+04    2.20133191E+04    2.20133191E+04    4.87694939E-01
 V20    -7.07096147E+00   -6.72498142E+00   -6.72498142E+00    1.27666146E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15868594E-01 TO   6.73924415E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.77348530E-03
PARROT: @@ Set alt mode to start
PARROT: s-alt Y
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV *alt*  1.0  1193.0      LIQUID A2B BCC
   2 AINV *alt*  1.0  1341.0      LIQUID A2B
   3 AINV *alt*  1.0  1049.0      LIQUID A2B BCC
   4 AINV *alt*  1.0  1203.0      LIQUID BCC FCC
   5 AINV *alt*  1.0   726.0      A2B BCC BCC#2
   6 AINV *alt*  1.0   726.0      BCC BCC#2
 Failed using alternate for FCC#1                      setting weight to zero
  10 ALF  *alt*  1.0  1594.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  11 ALF  *alt*  1.0  1548.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  12 ALF  *alt*  1.0  1499.0      LIQUID FCC
 Failed using alternate for FCC#1                      setting weight to zero
  13 ALF  *alt*  1.0  1438.0      LIQUID FCC
  20 ATIE *alt*  1.0  1413.0      LIQUID FCC
  21 ATIE *alt*  1.0  1337.0      LIQUID FCC
  22 ATIE *alt*  1.0  1213.0      LIQUID FCC
  23 ATIE *alt*  1.0  1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     2   1.    1773.0      LIQUID
 116 AH     2   1.    1773.0      LIQUID
 117 AH     2   1.    1773.0      LIQUID
 118 AH     2   1.    1773.0      LIQUID
 Number of alternate equilibria                    14
ED_EXP: @@ Equilibra with label ALF cannot use alt mode
ED_EXP: s-we 0 alf
 Changed weight on                      4 equilibria.
ED_EXP: c-a
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: save
ED_EXP: @@ Save changes of weights before leaving the editor
ED_EXP: ba
PARROT: @@ Optimize zero times as a check
PARROT: opt 0
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:50:55



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==
```

```
 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820940E+04    2.01820940E+04    3.02498609E-02
 V2     -2.94290453E+01   -2.90936148E+01   -2.90936148E+01    2.30117886E-02
 V11    -2.17328114E+04   -2.18127452E+04   -2.18127452E+04    3.47139480E-02
 V12     1.52102756E+01    1.55559538E+01    1.55559538E+01    5.38555607E-02
 V15     2.42012671E+04    2.36701118E+04    2.36701118E+04    8.60925907E-02
 V16    -8.38545766E+00   -7.56541436E+00   -7.56541436E+00    2.83695257E-01
 V17     3.08774212E+03    3.00342376E+03    3.00342376E+03    2.37803061E-01
 V19     2.20600544E+04    2.20133191E+04    2.20133191E+04    4.87694939E-01
 V20    -7.07096147E+00   -6.72498142E+00   -6.72498142E+00    1.27666146E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15868594E-01 TO   8.89279104E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   2.34020817E-03

 Number of alternate equilibria                    10


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                        0.00
   2 Alternate equilibrium calc                                        0.19
2 HTR=3727                        3714.      5.00E+02  -12.89     -2.5772E-02
   3 Alternate equilibrium calc                                        0.00
   4 Alternate equilibrium calc                                        0.00
   5 Alternate equilibrium calc                                        0.01
   6 Alternate equilibrium calc                                        0.01
  20 Alternate equilibrium calc                                        0.01
  21 Alternate equilibrium calc                                        0.00
  22 Alternate equilibrium calc                                        0.01
  23 Alternate equilibrium calc                                        0.00
100 ACR(B)=0.94                  0.9397      2.85E-02 -2.7309E-04 -9.5946E-03
101 ACR(B)=0.84                  0.8395      2.82E-02 -4.7482E-04 -1.6846E-02
102 ACR(B)=0.74                  0.7408      2.81E-02  7.6893E-04  2.7408E-02
103 ACR(B)=0.64                  0.6424      2.81E-02  2.4411E-03  8.6976E-02
104 ACR(B)=0.54                  0.5435      2.82E-02  3.5079E-03  0.1243
105 ACR(B)=0.44                  0.4429      2.85E-02  2.9003E-03  0.1016
106 ACR(B)=0.34                  0.3395      2.90E-02 -5.0467E-04 -1.7386E-02
107 ACR(B)=0.23                  0.2321      2.97E-02  2.0948E-03  7.0520E-02
108 ACR(B)=0.12                  0.1194      3.06E-02 -5.9712E-04 -1.9513E-02
110 HMR(LIQUID)=-1964            -1956.      5.00E+02   8.047      1.6094E-02
111 HMR(LIQUID)=-3500            -3477.      5.00E+02   22.75      4.5500E-02
112 HMR(LIQUID)=-4588            -4564.      5.00E+02   24.11      4.8219E-02
113 HMR(LIQUID)=-5239            -5216.      5.00E+02   23.13      4.6251E-02
114 HMR(LIQUID)=-5454            -5433.      5.00E+02   20.80      4.1594E-02
115 HMR(LIQUID)=-5233            -5216.      5.00E+02   17.13      3.4251E-02
116 HMR(LIQUID)=-4575            -4564.      5.00E+02   11.11      2.2219E-02
117 HMR(LIQUID)=-3481            -3477.      5.00E+02   3.750      7.5004E-03
118 HMR(LIQUID)=-1950            -1956.      5.00E+02  -5.953     -1.1906E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Note only one error from alternate calculations.
PARROT: @@ This error represents the difference in chemical
PARROT: @@ potentials of the phases.
PARROT: @@ Experiments with just one phase is calculated as normal.
PARROT: @@ Next command supresses the listing of parameters.
PARROT: s-o-l 1 Y Y N n N
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:50:55



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03691169E+04    2.01820940E+04    2.01820940E+04    3.02498609E-02
 V2     -2.94290453E+01   -2.90936148E+01   -2.90936148E+01    2.30117886E-02
 V11    -2.17328114E+04   -2.18127452E+04   -2.18127452E+04    3.47139480E-02
 V12     1.52102756E+01    1.55559538E+01    1.55559538E+01    5.38555607E-02
 V15     2.42012671E+04    2.36701118E+04    2.36701118E+04    8.60925907E-02
 V16    -8.38545766E+00   -7.56541436E+00   -7.56541436E+00    2.83695257E-01
 V17     3.08774212E+03    3.00342376E+03    3.00342376E+03    2.37803061E-01
 V19     2.20600544E+04    2.20133191E+04    2.20133191E+04    4.87694939E-01
 V20    -7.07096147E+00   -6.72498142E+00   -6.72498142E+00    1.27666146E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.15868594E-01 TO   8.89279104E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   2.34020817E-03

 Number of alternate equilibria                    10
```

```
 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20369.1168892663     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.4290452784981     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21732.8113609096     ; 6000 N REF0 !
 FUNCTION V12        298.15    15.2102756122622     ; 6000 N REF0 !
 FUNCTION V15        298.15    24201.2670828885     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.38545765692878     ; 6000 N REF0 !
 FUNCTION V17        298.15    3087.74212354332     ; 6000 N REF0 !
 FUNCTION V19        298.15    22060.0544125133     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.07096147078024     ; 6000 N REF0 !



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                        0.00
   2 Alternate equilibrium calc                                        0.19
2 HTR=3727                        3714.      5.00E+02  -12.89     -2.5772E-02
   3 Alternate equilibrium calc                                        0.00
   4 Alternate equilibrium calc                                        0.00
   5 Alternate equilibrium calc                                        0.01
   6 Alternate equilibrium calc                                        0.01
  20 Alternate equilibrium calc                                        0.01
  21 Alternate equilibrium calc                                        0.00
  22 Alternate equilibrium calc                                        0.01
  23 Alternate equilibrium calc                                        0.00
100 ACR(B)=0.94                  0.9397      2.85E-02 -2.7309E-04 -9.5946E-03
101 ACR(B)=0.84                  0.8395      2.82E-02 -4.7482E-04 -1.6846E-02
102 ACR(B)=0.74                  0.7408      2.81E-02  7.6893E-04  2.7408E-02
103 ACR(B)=0.64                  0.6424      2.81E-02  2.4411E-03  8.6976E-02
104 ACR(B)=0.54                  0.5435      2.82E-02  3.5079E-03  0.1243
105 ACR(B)=0.44                  0.4429      2.85E-02  2.9003E-03  0.1016
106 ACR(B)=0.34                  0.3395      2.90E-02 -5.0467E-04 -1.7386E-02
107 ACR(B)=0.23                  0.2321      2.97E-02  2.0948E-03  7.0520E-02
108 ACR(B)=0.12                  0.1194      3.06E-02 -5.9712E-04 -1.9513E-02
110 HMR(LIQUID)=-1964            -1956.      5.00E+02   8.047      1.6094E-02
111 HMR(LIQUID)=-3500            -3477.      5.00E+02   22.75      4.5500E-02
112 HMR(LIQUID)=-4588            -4564.      5.00E+02   24.11      4.8219E-02
113 HMR(LIQUID)=-5239            -5216.      5.00E+02   23.13      4.6251E-02
114 HMR(LIQUID)=-5454            -5433.      5.00E+02   20.80      4.1594E-02
115 HMR(LIQUID)=-5233            -5216.      5.00E+02   17.13      3.4251E-02
116 HMR(LIQUID)=-4575            -4564.      5.00E+02   11.11      2.2219E-02
117 HMR(LIQUID)=-3481            -3477.      5.00E+02   3.750      7.5004E-03
118 HMR(LIQUID)=-1950            -1956.      5.00E+02  -5.953     -1.1906E-02


PARROT:
PARROT: @@ Now optimize
PARROT: opt 30
 Alternate calculation is on
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    8.89279104E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    8.89950293E-02
  1  1.0094E+00   2  1.0115E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    8.89370498E-02
  1  1.0093E+00   2  1.0116E+00   3  9.9634E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    8.79489890E-02
  1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0224E+00
  6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00
```

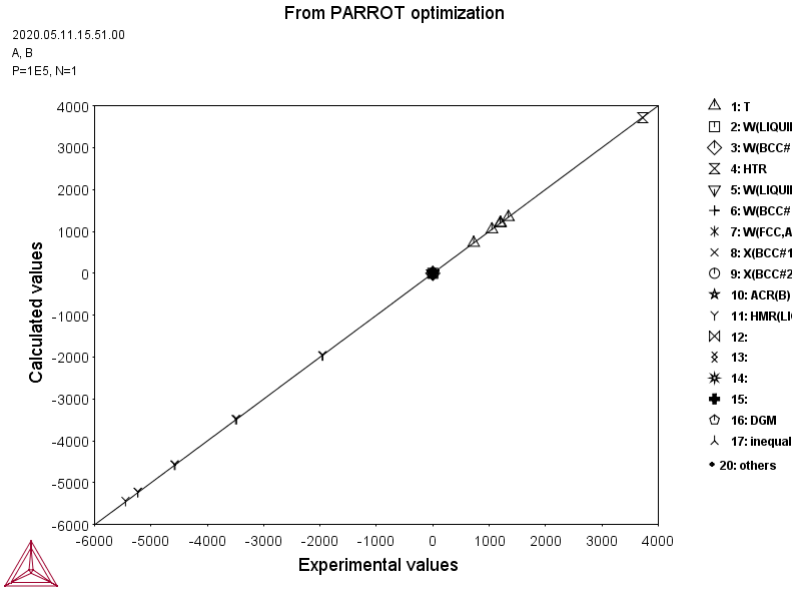
```
     AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    8.85893319E-02
 1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7788E-01   5  1.0224E+00
 6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79262645E-02
 1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
 6  1.1084E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79317667E-02
 1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
 6  1.1085E+00   7  1.0281E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79245155E-02
 1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
 6  1.1084E+00   7  1.0282E+00   8  1.0021E+00   9  1.0514E+00

     AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79198015E-02
 1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
 6  1.1084E+00   7  1.0282E+00   8  1.0022E+00   9  1.0514E+00

     AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    8.79216931E-02
 1  1.0093E+00   2  1.0115E+00   3  9.9644E-01   4  9.7778E-01   5  1.0225E+00
 6  1.1084E+00   7  1.0282E+00   8  1.0022E+00   9  1.0515E+00

     AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    6.30012578E-02
 1  1.0090E+00   2  1.0115E+00   3  1.0000E+00   4  9.7542E-01   5  1.0226E+00
 6  1.1084E+00   7  1.0282E+00   8  1.0022E+00   9  1.0514E+00

     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    6.00250624E-02
 1  1.0062E+00   2  1.0109E+00   3  9.9912E-01   4  9.7423E-01   5  1.0235E+00
 6  1.1105E+00   7  1.0290E+00   8  1.0016E+00   9  1.0501E+00

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    5.93161832E-02
 1  1.0057E+00   2  1.0092E+00   3  9.9970E-01   4  9.7424E-01   5  1.0255E+00
 6  1.1178E+00   7  1.0318E+00   8  1.0004E+00   9  1.0481E+00

     AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88760574E-02
 1  1.0049E+00   2  1.0059E+00   3  9.9988E-01   4  9.7463E-01   5  1.0295E+00
 6  1.1320E+00   7  1.0370E+00   8  9.9745E-01   9  1.0425E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   13 iterations
 1  1.0049E+00   2  1.0059E+00   3  9.9988E-01   4  9.7463E-01   5  1.0295E+00
 6  1.1320E+00   7  1.0370E+00   8  9.9745E-01   9  1.0425E+00

 1  6.9039E-03   2  6.9039E-03   3  1.5738E-03   4  2.6800E-03   5  1.3310E-01
 6 -1.3983E-01   7 -1.4164E-03   8  7.6472E-03   9  7.6472E-03  10 -1.0560E-04
11  3.2960E-03  12  2.1369E-03  13  2.5829E-04  14  3.0760E-03  15  6.0633E-04
16  1.2976E-03  17  1.2976E-03  18  2.3669E-05  19  1.6822E-03  20  2.3669E-05
21  1.6822E-03  22 -2.0443E-03  23  1.7694E-03  24  3.4709E-03  25  3.3350E-04
26 -2.5368E-03  27  3.2555E-03  28 -1.4427E-03  29  3.8328E-03  30 -1.3478E-02
31 -3.0855E-02  32 -6.3336E-04  33  4.3684E-02  34  6.7408E-02  35  3.5765E-02
36 -8.4872E-02  37  1.1726E-02  38 -5.6892E-02  39  2.1632E-03  40  2.0735E-02
41  1.5714E-02  42  9.1018E-03  43  2.8977E-03  44 -2.8982E-03  45 -1.0286E-02
46 -1.7265E-02  47 -2.5837E-02

                THE SUM OF SQUARES IS   5.88760574E-02
PARROT: cont 30

 It is safe to CONTINUE only after TOO MANY ITERATIONS
 and no change in variables and experiments ...
 Now anything can happen ...

PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:50:55



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  14


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02809885E+04    2.01820940E+04    2.01820940E+04    7.95746926E-02
 V2     -2.92651700E+01   -2.90936148E+01   -2.90936148E+01    3.44415326E-01
 V11    -2.18102047E+04   -2.18127452E+04   -2.18127452E+04    3.96943914E-02
 V12     1.51613087E+01    1.55559538E+01    1.55559538E+01    5.70071558E-02
 V15     2.43675664E+04    2.36701118E+04    2.36701118E+04    6.28240505E-01
 V16    -8.56377506E+00   -7.56541436E+00   -7.56541436E+00    2.32375042E+00
 V17     3.11464865E+03    3.00342376E+03    3.00342376E+03    1.51251787E+00
 V19     2.19570767E+04    2.20133191E+04    2.20133191E+04    4.62338058E+00
 V20    -7.01093202E+00   -6.72498142E+00   -6.72498142E+00    1.17285879E+01

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.89279104E-02 TO   5.88760574E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.54936993E-03

 Number of alternate equilibria                     10

 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20280.9885244626     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.2651699698526     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21810.2046870529     ; 6000 N REF0 !
```

```
 FUNCTION V12        298.15    15.1613087031845     ; 6000 N REF0 !
 FUNCTION V15        298.15    24367.5664077225     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.56377505595115     ; 6000 N REF0 !
 FUNCTION V17        298.15    3114.64864607825     ; 6000 N REF0 !
 FUNCTION V19        298.15    21957.0766579059     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.01093202288031     ; 6000 N REF0 !


 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
   1 Alternate equilibrium calc                                        0.01
   2 Alternate equilibrium calc                                        0.19
2 HTR=3727                        3726.      5.00E+02 -0.7082     -1.4164E-03
   3 Alternate equilibrium calc                                        0.01
   4 Alternate equilibrium calc                                        0.00
   5 Alternate equilibrium calc                                        0.00
   6 Alternate equilibrium calc                                        0.00
  20 Alternate equilibrium calc                                        0.00
  21 Alternate equilibrium calc                                        0.00
  22 Alternate equilibrium calc                                        0.00
  23 Alternate equilibrium calc                                        0.00
100 ACR(B)=0.94                  0.9396      2.85E-02 -3.8404E-04 -1.3478E-02
101 ACR(B)=0.84                  0.8391      2.82E-02 -8.7121E-04 -3.0855E-02
102 ACR(B)=0.74                  0.7400      2.81E-02 -1.7806E-05 -6.3336E-04
103 ACR(B)=0.64                  0.6412      2.81E-02  1.2286E-03  4.3684E-02
104 ACR(B)=0.54                  0.5419      2.83E-02  1.9060E-03  6.7408E-02
105 ACR(B)=0.44                  0.4410      2.86E-02  1.0218E-03  3.5765E-02
106 ACR(B)=0.34                  0.3375      2.90E-02 -2.4631E-03 -8.4872E-02
107 ACR(B)=0.23                  0.2303      2.96E-02  3.4765E-04  1.1726E-02
108 ACR(B)=0.12                  0.1183      3.05E-02 -1.7336E-03 -5.6892E-02
110 HMR(LIQUID)=-1964            -1963.      5.00E+02   1.082      2.1632E-03
111 HMR(LIQUID)=-3500            -3490.      5.00E+02   10.37      2.0735E-02
112 HMR(LIQUID)=-4588            -4580.      5.00E+02   7.857      1.5714E-02
113 HMR(LIQUID)=-5239            -5234.      5.00E+02   4.551      9.1018E-03
114 HMR(LIQUID)=-5454            -5453.      5.00E+02   1.449      2.8977E-03
115 HMR(LIQUID)=-5233            -5234.      5.00E+02  -1.449     -2.8982E-03
116 HMR(LIQUID)=-4575            -4580.      5.00E+02  -5.143     -1.0286E-02
117 HMR(LIQUID)=-3481            -3490.      5.00E+02  -8.633     -1.7265E-02
118 HMR(LIQUID)=-1950            -1963.      5.00E+02  -12.92     -2.5837E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ The liquid data fits reasonably. Simplify its parameters.
PARROT: l-p-d liq


 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
PARROT: @@ Rescale the start values of the parameters to current values
PARROT: resc
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02809885E+04    2.02809885E+04    2.02809885E+04    0.00000000E+00
 V2     -2.92651700E+01   -2.92651700E+01   -2.92651700E+01    0.00000000E+00
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43675664E+04    2.43675664E+04    2.43675664E+04    0.00000000E+00
```

```
 V16    -8.56377506E+00   -8.56377506E+00   -8.56377506E+00    0.00000000E+00
 V17     3.11464865E+03    3.11464865E+03    3.11464865E+03    0.00000000E+00
 V19     2.19570767E+04    2.19570767E+04    2.19570767E+04    0.00000000E+00
 V20    -7.01093202E+00   -7.01093202E+00   -7.01093202E+00    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT:Hit RETURN to continue
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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:   6.817E-01  7.266E+02
  ** A2B
     BCC#1
  ** BCC#2

 Phase region boundary   4 at:   3.625E-01  7.266E+02
  ** A2B
```

```
    BCC#1
Calculated.                      15 equilibria

Phase region boundary   5 at:   3.778E-01  1.185E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.888E-01  1.185E+03
 ** LIQUID
    BCC#1
Calculated                      28 equilibria

Phase region boundary   7 at:   4.900E-01  1.185E+03
 ** LIQUID
    A2B
Calculated.                      33 equilibria

Phase region boundary   8 at:   6.482E-01  1.039E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.637E-01  1.039E+03
    A2B
 ** BCC#1
Calculated.                      10 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.259E-01  1.039E+03
    LIQUID
 ** BCC#1
Calculated.                       8 equilibria

Phase region boundary  11 at:   8.759E-01  1.204E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.811E-01  1.204E+03
    LIQUID
 ** FCC
Calculated                      32 equilibria

Phase region boundary  13 at:   9.361E-01  1.204E+03
    BCC#1
 ** FCC
Calculated                      20 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
```

```
    BCC#2
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   3.646E-01  7.700E+02
  ** A2B
    BCC#1
 Calculated                      10 equilibria

 Phase region boundary  26 at:   3.646E-01  7.700E+02
  ** A2B
    BCC#1
 Calculated.                       3 equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   3.646E-01  7.700E+02
  ** A2B
    BCC#1
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.909E-01  7.700E+02
  ** A2B
    BCC#1
 Calculated                      10 equilibria

 Phase region boundary  29 at:   7.909E-01  7.700E+02
  ** A2B
    BCC#1
 Calculated.                       3 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.909E-01  7.700E+02
  ** A2B
    BCC#1
 Calculated.                       9 equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.435E-01  1.230E+03
  ** LIQUID
    BCC#1
 Calculated.                       4 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.435E-01  1.230E+03
  ** LIQUID
    BCC#1
 Calculated                      26 equilibria

 Phase region boundary  33 at:   8.867E-01  1.230E+03
  ** LIQUID
    FCC
 Calculated.                       2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.867E-01  1.230E+03
  ** LIQUID
    FCC
 Calculated                      29 equilibria

 Phase region boundary  35 at:   6.404E-03  1.397E+03
    LIQUID
  ** BCC#1
 Calculated                      10 equilibria

 Phase region boundary  36 at:   6.404E-03  1.397E+03
    LIQUID
  ** BCC#1
 Calculated.                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.295E-01  1.243E+03
    LIQUID
  ** BCC#1
 Calculated                      22 equilibria

 Phase region boundary  38 at:   2.295E-01  1.243E+03
    LIQUID
  ** BCC#1
 Calculated.                       4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.215E+03
    LIQUID
  ** A2B
 Calculated.                      12 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.215E+03
    LIQUID
  ** A2B
 Calculated.                       8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
    LIQUID
  ** FCC
 Calculated.                      19 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
    LIQUID
  ** FCC
 Calculated                      13 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     1 seconds
POLY: post
POST: s-l d
POST: plot
```



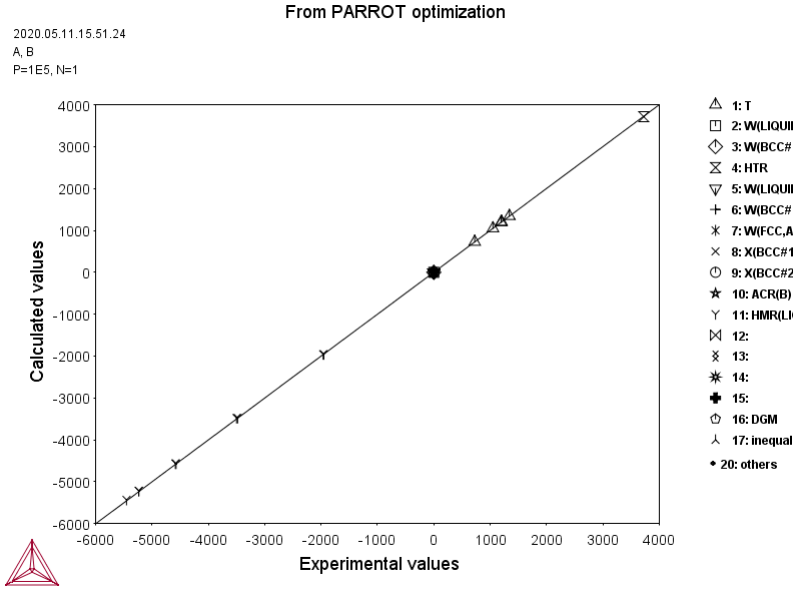

```
POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ This does not look very good, optimize more ...
PARROT: opt 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    5.88760574E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    5.88814906E-02
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    5.88785937E-02
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    5.88751228E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88749463E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88746803E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88754525E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88744380E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    7 iterations
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

  1  6.9039E-03   2  6.9039E-03   3  1.5746E-03   4  2.8286E-03   5  1.3310E-01
  6 -1.3983E-01   7 -1.4164E-03   8  7.6472E-03   9  7.6472E-03  10  1.9876E-06
 11  3.3001E-03  12  2.2286E-03  13  2.5992E-04  14  3.0133E-03  15  6.0473E-04
 16  1.1906E-03  17  1.1906E-03  18  2.3706E-04  19  1.3648E-03  20  2.3706E-04
 21  1.3648E-03  22 -2.1141E-03  23  1.7687E-03  24  3.4041E-03  25  3.3248E-04
 26 -2.5998E-03  27  3.2539E-03  28 -1.3406E-03  29  3.8359E-03  30 -1.3478E-02
 31 -3.0855E-02  32 -6.3336E-04  33  4.3684E-02  34  6.7408E-02  35  3.5765E-02
 36 -8.4872E-02  37  1.1726E-02  38 -5.6892E-02  39  2.1632E-03  40  2.0735E-02
 41  1.5714E-02  42  9.1018E-03  43  2.8977E-03  44 -2.8982E-03  45 -1.0286E-02
 46 -1.7265E-02  47 -2.5837E-02

                THE SUM OF SQUARES IS   5.88744380E-02
PARROT: resc
PARROT: opt 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    5.88744380E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    5.88798233E-02
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    5.88770246E-02
```

```
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    5.88744667E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88743605E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88740937E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

     AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88747823E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0000E+00

     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    5.88738859E-02
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    7 iterations
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

  1  6.9039E-03   2  6.9039E-03   3  1.5745E-03   4  2.7586E-03   5  1.3310E-01
  6 -1.3983E-01   7 -1.4164E-03   8  7.6472E-03   9  7.6472E-03  10 -6.7434E-05
 11  3.2926E-03  12  2.1470E-03  13  2.5560E-04  14  2.9506E-03  15  6.0313E-04
 16  1.2088E-03  17  1.2088E-03  18  1.3410E-04  19  1.4165E-03  20  1.3410E-04
 21  1.4165E-03  22 -2.1840E-03  23  1.7680E-03  24  3.3372E-03  25  3.3146E-04
 26 -2.6628E-03  27  3.2524E-03  28 -1.4140E-03  29  3.8295E-03  30 -1.3478E-02
 31 -3.0855E-02  32 -6.3336E-04  33  4.3684E-02  34  6.7408E-02  35  3.5765E-02
 36 -8.4872E-02  37  1.1726E-02  38 -5.6892E-02  39  2.1632E-03  40  2.0735E-02
 41  1.5714E-02  42  9.1018E-03  43  2.8977E-03  44 -2.8982E-03  45 -1.0286E-02
 46 -1.7265E-02  47 -2.5837E-02

               THE SUM OF SQUARES IS   5.88738859E-02
PARROT: @@ No change in the parameters, check the diagram again
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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:   6.817E-01  7.266E+02
 ** A2B
    BCC#1
 ** BCC#2

Phase region boundary   4 at:   3.625E-01  7.266E+02
 ** A2B
    BCC#1
Calculated.                      15 equilibria

Phase region boundary   5 at:   3.778E-01  1.185E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.887E-01  1.185E+03
 ** LIQUID
    BCC#1
Calculated                      25 equilibria

Phase region boundary   7 at:   4.900E-01  1.185E+03
 ** LIQUID
    A2B
Calculated.                      33 equilibria

Phase region boundary   8 at:   6.482E-01  1.039E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.637E-01  1.039E+03
    A2B
 ** BCC#1
Calculated.                      10 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.259E-01  1.039E+03
    LIQUID
 ** BCC#1
Calculated.                       8 equilibria

Phase region boundary  11 at:   8.758E-01  1.204E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.811E-01  1.204E+03
    LIQUID
 ** FCC
Calculated                      32 equilibria

Phase region boundary  13 at:   9.361E-01  1.204E+03
    BCC#1
 ** FCC
Calculated                      18 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
```

```
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.646E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                      10 equilibria

Phase region boundary  26 at:   3.646E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.646E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.909E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                      10 equilibria

Phase region boundary  29 at:   7.909E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.909E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.435E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.435E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated                      26 equilibria

Phase region boundary  33 at:   8.867E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.867E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                      29 equilibria

Phase region boundary  35 at:   6.404E-03  1.397E+03
    LIQUID
 ** BCC#1
Calculated                      11 equilibria

Phase region boundary  36 at:   6.404E-03  1.397E+03
    LIQUID
 ** BCC#1
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.295E-01  1.243E+03
    LIQUID
 ** BCC#1
Calculated                      22 equilibria

Phase region boundary  38 at:   2.295E-01  1.243E+03
    LIQUID
 ** BCC#1
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.215E+03
    LIQUID
```

```
 ** A2B
 Calculated.                      12 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.215E+03
     LIQUID
 ** A2B
 Calculated.                       8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
 ** FCC
 Calculated.                      19 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
 ** FCC
 Calculated                      14 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     1 seconds
POLY: post
POST: s-l d
POST: plot
```




```
POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Turn off alternate mode and try to calculate all equilibria
PARROT: s-alt Y
 Alternate calculation is on
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   3   1.    1184.6      LIQUID A2B BCC
   2 AINV   2   1.    1314.5      LIQUID A2B
   3 AINV   3   1.    1039.0      LIQUID A2B BCC
   4 AINV   3   1.    1204.2      LIQUID BCC FCC
   5 AINV   3   1.     726.6      A2B BCC BCC#2
   6 AINV   3   1.     726.0      BCC BCC#2
  10 ALF  < unused >  1594.0      LIQUID FCC
  11 ALF  < unused >  1548.0      LIQUID FCC
  12 ALF  < unused >  1499.0      LIQUID FCC
  13 ALF  < unused >  1438.0      LIQUID FCC
  20 ATIE   3   1.    1413.0      LIQUID FCC
  21 ATIE   3   1.    1337.0      LIQUID FCC
  22 ATIE   3   1.    1213.0      LIQUID FCC
  23 ATIE   3   1.    1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 115 AH     2   1.    1773.0      LIQUID
 116 AH     2   1.    1773.0      LIQUID
 117 AH     2   1.    1773.0      LIQUID
 118 AH     2   1.    1773.0      LIQUID
ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
ED_EXP: @@ any liquid parameters and restore those with label ALF
ED_EXP: s-we 0 100-118
ED_EXP: s-we 1 alf
 Changed weight on                       4 equilibria.
ED_EXP: s-e 1
 Equilibrium number                       1, label AINV
ED_EXP: c-a
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
```

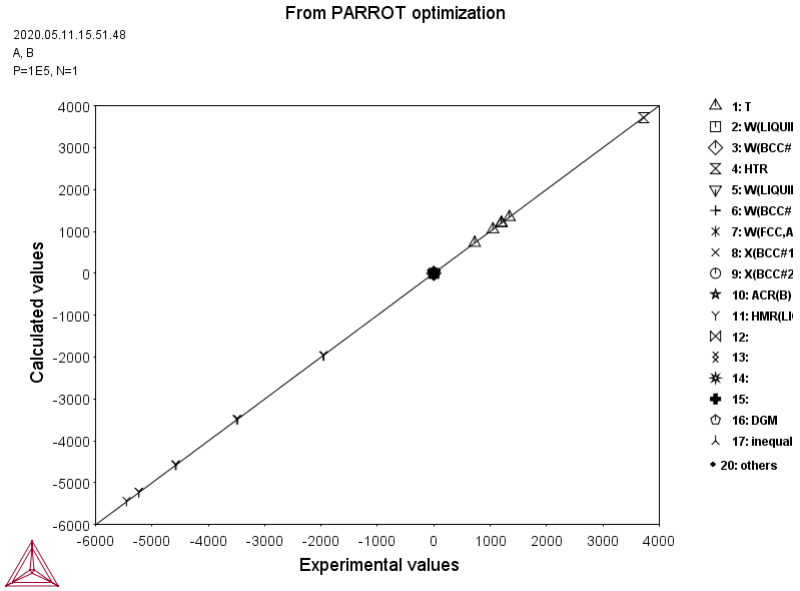
```
  1 AINV   2   1.    1184.6      LIQUID A2B BCC
  2 AINV   2   1.    1314.5      LIQUID A2B
  3 AINV   2   1.    1039.0      LIQUID A2B BCC
  4 AINV   2   1.    1204.2      LIQUID BCC FCC
  5 AINV   2   1.     726.6      A2B BCC BCC#2
  6 AINV   2   1.     726.0      BCC BCC#2
 10 ALF    3   1.    1594.0      LIQUID FCC
 11 ALF    3   1.    1548.0      LIQUID FCC
 12 ALF    3   1.    1499.0      LIQUID FCC
 13 ALF    3   1.    1438.0      LIQUID FCC
 20 ATIE   2   1.    1413.0      LIQUID FCC
 21 ATIE   2   1.    1337.0      LIQUID FCC
 22 ATIE   2   1.    1213.0      LIQUID FCC
 23 ATIE   2   1.    1100.0      LIQUID BCC
100 AA   < unused >  1573.0      LIQUID
101 AA   < unused >  1573.0      LIQUID
102 AA   < unused >  1573.0      LIQUID
103 AA   < unused >  1573.0      LIQUID
104 AA   < unused >  1573.0      LIQUID
105 AA   < unused >  1573.0      LIQUID
106 AA   < unused >  1573.0      LIQUID
107 AA   < unused >  1573.0      LIQUID
108 AA   < unused >  1573.0      LIQUID
110 AH   < unused >  1773.0      LIQUID
111 AH   < unused >  1773.0      LIQUID
112 AH   < unused >  1773.0      LIQUID
113 AH   < unused >  1773.0      LIQUID
114 AH   < unused >  1773.0      LIQUID
115 AH   < unused >  1773.0      LIQUID
116 AH   < unused >  1773.0      LIQUID
117 AH   < unused >  1773.0      LIQUID
118 AH   < unused >  1773.0      LIQUID
ED_EXP: save
ED_EXP: @@ Save changes
ED_EXP: ba
PARROT: opt 0
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r C SCREEN


          ==================================================
          OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:51:46



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02809885E+04    2.02809885E+04    2.02809885E+04    7.39143651E-02
 V2     -2.92651700E+01   -2.92651700E+01   -2.92651700E+01    3.41787473E-01
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43700032E+04    2.43700032E+04    2.43700032E+04    6.09487675E-01
 V16    -8.56548790E+00   -8.56463143E+00   -8.56463143E+00    2.04922290E+00
 V17     3.11527161E+03    3.11496011E+03    3.11496011E+03    1.45833484E+00
 V19     2.19570767E+04    2.19570767E+04    2.19570767E+04    4.63522311E+00
 V20    -7.01233428E+00   -7.01163312E+00   -7.01163312E+00    1.12486772E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.88744380E-02 TO   8.99442541E+00
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   4.08837519E-01


 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20280.9885244626     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.2651699698526     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21810.2046870529     ; 6000 N REF0 !
 FUNCTION V12        298.15    15.1613087031845     ; 6000 N REF0 !
 FUNCTION V15        298.15    24370.0031643633     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.56548789660009     ; 6000 N REF0 !
 FUNCTION V17        298.15    3115.27160695395     ; 6000 N REF0 !
 FUNCTION V19        298.15    21957.0766579059     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.01233427939421     ; 6000 N REF0 !



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)
```

```
 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1185.       10.      -8.445     -0.8445
1 W(LIQUID,B)=0.408              0.4163      2.00E-02  8.3025E-03  0.4151
1 W(BCC#1,B)=0.13                0.1322      2.00E-02  2.2006E-03  0.1100
2 T=1341                          1315.       10.      -26.49      -2.649
2 HTR=3727                        3726.      5.00E+02 -0.7083     -1.4167E-03
3 T=1049                          1039.       10.      -10.03      -1.003
3 W(LIQUID,A)=0.27               0.2735      2.00E-02  3.4728E-03  0.1736
3 W(BCC#1,A)=9.3E-2              9.3787E-02  2.00E-02  7.8737E-04  3.9368E-02
4 T=1203                          1204.       10.       1.179      0.1179
4 W(LIQUID,A)=0.19               0.1890      2.00E-02 -9.8135E-04 -4.9067E-02
4 W(BCC#1,A)=6.9E-2              6.8455E-02  2.00E-02 -5.4511E-04 -2.7255E-02
4 W(FCC,A)=6E-2                  5.9376E-02  2.00E-02 -6.2387E-04 -3.1194E-02
5 T=726                           726.6       10.      0.6276      6.2757E-02
5 X(BCC#1,B)=3.7E-2              3.7255E-02  2.00E-02  2.5471E-04  1.2736E-02
5 X(BCC#2,A)=0.114               0.1144      2.00E-02  4.0100E-04  2.0050E-02
6 X(BCC#1,B)=3.7E-2              3.7078E-02  2.00E-02  7.8114E-05  3.9057E-03
6 X(BCC#2,A)=0.114               0.1140      2.00E-02 -3.4069E-05 -1.7035E-03
10 W(LIQUID,A)=2E-2              1.9384E-02  2.00E-02 -6.1575E-04 -3.0788E-02
11 W(LIQUID,A)=4.2E-2            4.1484E-02  2.00E-02 -5.1605E-04 -2.5802E-02
12 W(LIQUID,A)=6.5E-2            6.4387E-02  2.00E-02 -6.1266E-04 -3.0633E-02
13 W(LIQUID,A)=9.3E-2            9.2002E-02  2.00E-02 -9.9776E-04 -4.9888E-02
20 W(LIQUID,A)=0.104             0.1030      2.00E-02 -9.6497E-04 -4.8249E-02
20 W(FCC,A)=3.8E-2               3.7713E-02  2.00E-02 -2.8716E-04 -1.4358E-02
21 W(LIQUID,A)=0.136             0.1356      2.00E-02 -4.2474E-04 -2.1237E-02
21 W(FCC,A)=4.7E-2               4.6609E-02  2.00E-02 -3.9077E-04 -1.9538E-02
22 W(LIQUID,A)=0.187             0.1856      2.00E-02 -1.4041E-03 -7.0205E-02
22 W(FCC,A)=5.9E-2               5.8614E-02  2.00E-02 -3.8608E-04 -1.9304E-02
23 W(LIQUID,A)=0.245             0.2434      2.00E-02 -1.5869E-03 -7.9345E-02
23 W(BCC#1,A)=8.5E-2             8.4361E-02  2.00E-02 -6.3921E-04 -3.1960E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for
PARROT: @@ equilibrium 4. It can be on the wrong side, at high A instead
PARROT: @@  of high B. Try to correct that in the Edit module.
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
 Equilibrium number                      4, label AINV
ED_EXP: s-a-s
T /1204.179215/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
 Testing result with global minimization
    13 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=1   FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1204.18 K (   931.03 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.30210E+02
 Total Gibbs energy -9.82098E+03,  Enthalpy  1.98581E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.5966E-01  1.0132E-01 3.8855E-01 -9.4648E+03 SER
 B                       2.3403E+00  8.9868E-01 8.5841E-01 -1.5286E+03 SER

 FCC                         Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5911E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.40624E-01  A  5.93761E-02

 BCC#1                       Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5344E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.31545E-01  A  6.84549E-02

 LIQUID                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.8955E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.10981E-01  A  1.89019E-01
```

```
 EXPERIMENT T=1203:DT  $1204.18:10  NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX  $0.189019:2E-2  NO=2
 EXPERIMENT W(BCC#1,A)=6.9E-2:DX  $6.84549E-2:2E-2  NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX  $5.93761E-2:2E-2  NO=4
ED_EXP: ba
PARROT: @@ The error is still there, calculate the phase diagram.
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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:   6.817E-01  7.266E+02
  ** A2B
     BCC#1
  ** BCC#2

 Phase region boundary   4 at:   3.625E-01  7.266E+02
  ** A2B
     BCC#1
 Calculated.                      15 equilibria
```

```
Phase region boundary   5 at:   3.778E-01  1.185E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.887E-01  1.185E+03
 ** LIQUID
    BCC#1
Calculated                      25 equilibria

Phase region boundary   7 at:   4.900E-01  1.185E+03
 ** LIQUID
    A2B
Calculated.                      33 equilibria

Phase region boundary   8 at:   6.482E-01  1.039E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.637E-01  1.039E+03
    A2B
 ** BCC#1
Calculated.                      10 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.259E-01  1.039E+03
    LIQUID
 ** BCC#1
Calculated.                       8 equilibria

Phase region boundary  11 at:   8.758E-01  1.204E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.811E-01  1.204E+03
    LIQUID
 ** FCC
Calculated                      32 equilibria

Phase region boundary  13 at:   9.361E-01  1.204E+03
    BCC#1
 ** FCC
Calculated                      18 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
```

```
 Terminating at known equilibrium

 Phase region boundary  25 at:   3.646E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                     10 equilibria

 Phase region boundary  26 at:   3.646E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                     3 equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   3.646E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                    13 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.909E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                     10 equilibria

 Phase region boundary  29 at:   7.909E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                     3 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.909E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                     9 equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.435E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated.                     4 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.435E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated                     26 equilibria

 Phase region boundary  33 at:   8.867E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                     2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.867E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                     29 equilibria

 Phase region boundary  35 at:   6.404E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated                     11 equilibria

 Phase region boundary  36 at:   6.404E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated.                    13 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.295E-01  1.243E+03
     LIQUID
  ** BCC#1
 Calculated                     22 equilibria

 Phase region boundary  38 at:   2.295E-01  1.243E+03
     LIQUID
  ** BCC#1
 Calculated.                     4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.215E+03
     LIQUID
  ** A2B
 Calculated.                    12 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.215E+03
     LIQUID
  ** A2B
 Calculated.                     8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                    19 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                     14 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     1 seconds
POLY: post
POST: s-l d
POST: plot
```




```
POST:
POST: set-inter
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
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: ed
ED_EXP: read 1
ED_EXP: s-we 0 4
ED_EXP: save
ED_EXP: ba
PARROT: opt 0
 Use      25 experiments, maximum is        2000
 Use     494 real workspace, maximum is    50000
PARROT: l-r C SCREEN


            ==================================================
            OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:52:10



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.02809885E+04    2.02809885E+04    2.02809885E+04    7.39143651E-02
 V2     -2.92651700E+01   -2.92651700E+01   -2.92651700E+01    3.41787473E-01
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43700032E+04    2.43700032E+04    2.43700032E+04    6.09487675E-01
 V16    -8.56548790E+00   -8.56463143E+00   -8.56463143E+00    2.04922290E+00
 V17     3.11527161E+03    3.11496011E+03    3.11496011E+03    1.45833484E+00
 V19     2.19570767E+04    2.19570767E+04    2.19570767E+04    4.63522311E+00
 V20    -7.01233428E+00   -7.01163312E+00   -7.01163312E+00    1.12486772E+01

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   5.88744380E-02 TO   8.97639645E+00
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   4.98688691E-01


 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20280.9885244626     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.2651699698526     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21810.2046870529     ; 6000 N REF0 !
 FUNCTION V12        298.15    15.1613087031845     ; 6000 N REF0 !
 FUNCTION V15        298.15    24370.0031643633     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.56548789660009     ; 6000 N REF0 !
 FUNCTION V17        298.15    3115.27160695395     ; 6000 N REF0 !
 FUNCTION V19        298.15    21957.0766579059     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.01233427939421     ; 6000 N REF0 !
```

```
 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1185.       10.      -8.445     -0.8445
1 W(LIQUID,B)=0.408              0.4163      2.00E-02  8.3025E-03  0.4151
1 W(BCC#1,B)=0.13                0.1322      2.00E-02  2.2006E-03  0.1100
2 T=1341                          1315.       10.      -26.49      -2.649
2 HTR=3727                        3726.      5.00E+02 -0.7083     -1.4167E-03
3 T=1049                          1039.       10.      -10.03      -1.003
3 W(LIQUID,A)=0.27               0.2735      2.00E-02  3.4728E-03  0.1736
3 W(BCC#1,A)=9.3E-2              9.3787E-02  2.00E-02  7.8737E-04  3.9368E-02
5 T=726                           726.6       10.      0.6276      6.2757E-02
5 X(BCC#1,B)=3.7E-2              3.7255E-02  2.00E-02  2.5471E-04  1.2736E-02
5 X(BCC#2,A)=0.114               0.1144      2.00E-02  4.0100E-04  2.0050E-02
6 X(BCC#1,B)=3.7E-2              3.7078E-02  2.00E-02  7.8114E-05  3.9057E-03
6 X(BCC#2,A)=0.114               0.1140      2.00E-02 -3.4069E-05 -1.7035E-03
10 W(LIQUID,A)=2E-2              1.9384E-02  2.00E-02 -6.1575E-04 -3.0788E-02
11 W(LIQUID,A)=4.2E-2            4.1484E-02  2.00E-02 -5.1605E-04 -2.5802E-02
12 W(LIQUID,A)=6.5E-2            6.4387E-02  2.00E-02 -6.1266E-04 -3.0633E-02
13 W(LIQUID,A)=9.3E-2            9.2002E-02  2.00E-02 -9.9776E-04 -4.9888E-02
20 W(LIQUID,A)=0.104             0.1030      2.00E-02 -9.6497E-04 -4.8249E-02
20 W(FCC,A)=3.8E-2               3.7713E-02  2.00E-02 -2.8716E-04 -1.4358E-02
21 W(LIQUID,A)=0.136             0.1356      2.00E-02 -4.2474E-04 -2.1237E-02
21 W(FCC,A)=4.7E-2               4.6609E-02  2.00E-02 -3.9077E-04 -1.9538E-02
22 W(LIQUID,A)=0.187             0.1856      2.00E-02 -1.4041E-03 -7.0205E-02
22 W(FCC,A)=5.9E-2               5.8614E-02  2.00E-02 -3.8608E-04 -1.9304E-02
23 W(LIQUID,A)=0.245             0.2434      2.00E-02 -1.5869E-03 -7.9345E-02
23 W(BCC#1,A)=8.5E-2             8.4361E-02  2.00E-02 -6.3921E-04 -3.1960E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 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    8.97639645E+00
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    9.13899280E+00
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    8.68323978E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    8.69025565E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0001E+00   4  1.0001E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    8.68060743E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0002E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    8.68024407E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0002E+00   5  1.0002E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    8.68060536E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0002E+00   5  1.0002E+00
  6  1.0001E+00   7  1.0001E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    8.68009183E+00
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0002E+00   5  1.0002E+00
  6  1.0000E+00   7  1.0002E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    4.74733291E-01
  1  9.9763E-01   2  1.0044E+00   3  9.9990E-01   4  1.0002E+00   5  1.0002E+00
  6  9.9999E-01   7  1.0002E+00
```

```
     AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    3.94612068E-01
 1  9.9883E-01   2  1.0048E+00   3  9.9988E-01   4  1.0031E+00   5  1.0015E+00
 6  1.0010E+00   7  1.0037E+00

     AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    3.39925235E-01
 1  9.9933E-01   2  1.0054E+00   3  1.0002E+00   4  1.0049E+00   5  1.0023E+00
 6  1.0045E+00   7  1.0127E+00

     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    2.09925938E-01
 1  1.0023E+00   2  1.0068E+00   3  1.0020E+00   4  1.0149E+00   5  1.0070E+00
 6  9.9722E-01   7  9.9852E-01

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27915999E-01
 1  1.0072E+00   2  1.0096E+00   3  1.0064E+00   4  1.0333E+00   5  1.0153E+00
 6  1.0040E+00   7  1.0210E+00

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   12 iterations
 1  1.0072E+00   2  1.0096E+00   3  1.0064E+00   4  1.0333E+00   5  1.0153E+00
 6  1.0040E+00   7  1.0210E+00

 1 -1.2012E-01   2  1.6807E-02   3  7.7726E-02   4  7.5285E-02   5 -9.8949E-02
 6 -1.6451E-01   7  5.6332E-02   8  1.1680E-01   9 -1.5429E-01  10 -1.7636E-02
11  3.4908E-02  12  4.0882E-03  13  8.9192E-02  14 -2.2047E-02  15 -9.2885E-03
16 -8.1454E-03  17 -2.2546E-02  18 -1.9582E-02  19  1.7801E-02  20  9.6277E-03
21  1.8367E-02  22 -3.9899E-02  23  2.5880E-02  24  9.1761E-03  25  9.9469E-02

              THE SUM OF SQUARES IS   1.27915999E-01
```

PARROT: cont 30

```
 It is safe to CONTINUE only after TOO MANY ITERATIONS
 and no change in variables and experiments ...
 Now anything can happen ...
```

PARROT: l-r C SCREEN

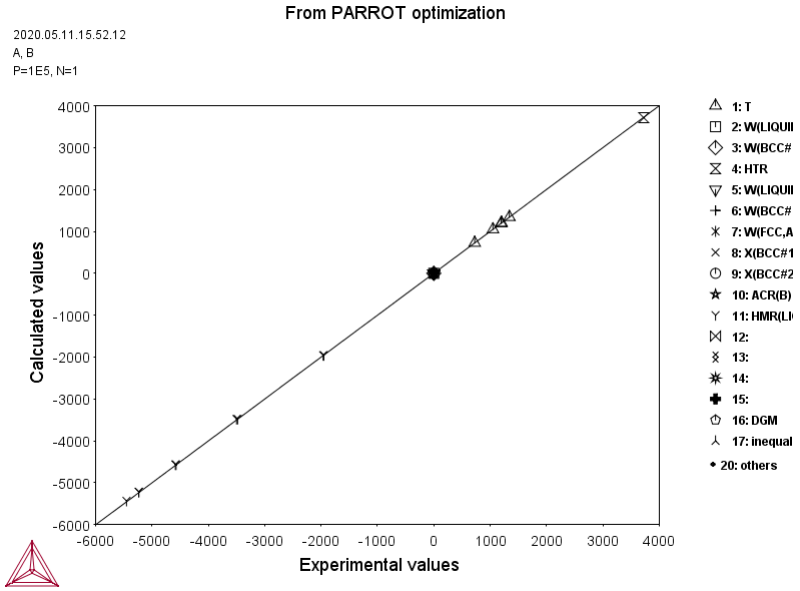
```
          ==================================================
          OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:52:10



 *** 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      2.04272875E+04    2.02809885E+04    2.02809885E+04    2.59209707E-02
 V2     -2.95468613E+01   -2.92651700E+01   -2.92651700E+01    1.40177728E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.45250655E+04    2.43700032E+04    2.43700032E+04    9.62418615E-02
 V16    -8.85015065E+00   -8.56463143E+00   -8.56463143E+00    2.78844065E-01
 V17     3.16252981E+03    3.11496011E+03    3.11496011E+03    2.49147762E-01
 V19     2.20441096E+04    2.19570767E+04    2.19570767E+04    6.73748369E-01
 V20    -7.15892204E+00   -7.01163312E+00   -7.01163312E+00    1.60351724E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.97639645E+00 TO   1.27915999E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   7.10644438E-03


 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20427.2875080025     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.5468612774370     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21810.2046870529     ; 6000 N REF0 !
 FUNCTION V12        298.15    15.1613087031845     ; 6000 N REF0 !
 FUNCTION V15        298.15    24525.0654991989     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.85015065440329     ; 6000 N REF0 !
 FUNCTION V17        298.15    3162.52981307340     ; 6000 N REF0 !
 FUNCTION V19        298.15    22044.1096459343     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.15892204220753     ; 6000 N REF0 !



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B
```

```
      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.       10.      -1.201     -0.1201
1 W(LIQUID,B)=0.408              0.4083      2.00E-02  3.3615E-04  1.6807E-02
1 W(BCC#1,B)=0.13                0.1316      2.00E-02  1.5545E-03  7.7726E-02
2 T=1341                          1342.       10.      0.7529      7.5285E-02
2 HTR=3727                        3678.      5.00E+02  -49.47     -9.8949E-02
3 T=1049                          1047.       10.      -1.645     -0.1645
3 W(LIQUID,A)=0.27               0.2711      2.00E-02  1.1266E-03  5.6332E-02
3 W(BCC#1,A)=9.3E-2              9.5336E-02  2.00E-02  2.3361E-03  0.1168
5 T=726                           724.5       10.      -1.543     -0.1543
5 X(BCC#1,B)=3.7E-2              3.6647E-02  2.00E-02 -3.5272E-04 -1.7636E-02
5 X(BCC#2,A)=0.114               0.1147      2.00E-02  6.9816E-04  3.4908E-02
6 X(BCC#1,B)=3.7E-2              3.7082E-02  2.00E-02  8.1763E-05  4.0882E-03
6 X(BCC#2,A)=0.114               0.1158      2.00E-02  1.7838E-03  8.9192E-02
10 W(LIQUID,A)=2E-2              1.9559E-02  2.00E-02 -4.4094E-04 -2.2047E-02
11 W(LIQUID,A)=4.2E-2            4.1814E-02  2.00E-02 -1.8577E-04 -9.2885E-03
12 W(LIQUID,A)=6.5E-2            6.4837E-02  2.00E-02 -1.6291E-04 -8.1454E-03
13 W(LIQUID,A)=9.3E-2            9.2549E-02  2.00E-02 -4.5092E-04 -2.2546E-02
20 W(LIQUID,A)=0.104             0.1036      2.00E-02 -3.9164E-04 -1.9582E-02
20 W(FCC,A)=3.8E-2               3.8356E-02  2.00E-02  3.5602E-04  1.7801E-02
21 W(LIQUID,A)=0.136             0.1362      2.00E-02  1.9255E-04  9.6277E-03
21 W(FCC,A)=4.7E-2               4.7367E-02  2.00E-02  3.6734E-04  1.8367E-02
22 W(LIQUID,A)=0.187             0.1862      2.00E-02 -7.9799E-04 -3.9899E-02
22 W(FCC,A)=5.9E-2               5.9518E-02  2.00E-02  5.1760E-04  2.5880E-02
23 W(LIQUID,A)=0.245             0.2452      2.00E-02  1.8352E-04  9.1761E-03
23 W(BCC#1,A)=8.5E-2             8.6989E-02  2.00E-02  1.9894E-03  9.9469E-02


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Optimization converged, try to add equilibrium 4 again
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
 Equilibrium number                      4, label AINV
ED_EXP: s-a-s
T /1204.179215/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
 Testing result with global minimization
    13 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=1   FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1211.83 K (   938.68 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.30242E+02
 Total Gibbs energy -1.00413E+04,  Enthalpy  1.99592E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.5860E-01  1.0113E-01 3.8288E-01 -9.6731E+03 SER
 B                       2.3414E+00  8.9887E-01 8.5591E-01 -1.5677E+03 SER

 FCC                        Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5896E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.40380E-01  A  5.96204E-02

 BCC#1                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5283E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.30563E-01  A  6.94370E-02

 LIQUID                     Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.9063E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.13344E-01  A  1.86656E-01
 SET_WEIGHT 0,,,
 EXPERIMENT T=1203:DT
 EXPERIMENT W(LIQUID,A)=0.19:DX
 EXPERIMENT W(BCC#1,A)=6.9E-2:DX
 EXPERIMENT W(FCC,A)=6E-2:DX
ED_EXP: ba
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
```

```
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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:   6.813E-01  7.245E+02
  ** A2B
     BCC#1
  ** BCC#2

 Phase region boundary   4 at:   3.620E-01  7.245E+02
  ** A2B
     BCC#1
 Calculated.                      15 equilibria

 Phase region boundary   5 at:   3.775E-01  1.192E+03
  ** LIQUID
  ** A2B
     BCC#1

 Phase region boundary   6 at:   2.837E-01  1.192E+03
  ** LIQUID
     BCC#1
 Calculated                      24 equilibria
```

```
Phase region boundary   7 at:   4.865E-01  1.192E+03
 ** LIQUID
    A2B
Calculated.                     33 equilibria

Phase region boundary   8 at:   6.495E-01  1.047E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.626E-01  1.047E+03
    A2B
 ** BCC#1
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.259E-01  1.047E+03
    LIQUID
 ** BCC#1
Calculated.                      9 equilibria

Phase region boundary  11 at:   8.763E-01  1.212E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.820E-01  1.212E+03
    LIQUID
 ** FCC
Calculated                     35 equilibria

Phase region boundary  13 at:   9.355E-01  1.212E+03
    BCC#1
 ** FCC
Calculated                     24 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                     2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.642E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                     10 equilibria

Phase region boundary  26 at:   3.642E-01  7.700E+02
 ** A2B
    BCC#1
```

```
 Calculated.                      3 equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   3.642E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                     14 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.905E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                      10 equilibria

 Phase region boundary  29 at:   7.905E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                      3 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.905E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                      9 equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.451E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated.                      4 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.451E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated                      26 equilibria

 Phase region boundary  33 at:   8.859E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                      2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.859E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                      29 equilibria

 Phase region boundary  35 at:   6.428E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated                       8 equilibria

 Phase region boundary  36 at:   6.428E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated.                     13 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.303E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated                      22 equilibria

 Phase region boundary  38 at:   2.303E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated.                      4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.239E+03
     LIQUID
  ** A2B
 Calculated.                     14 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.239E+03
     LIQUID
  ** A2B
 Calculated.                      8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                     19 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                       9 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                      1 seconds
POLY: post
POST: s-l d
POST: plot
```




```
POST:
POST: set-inter
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
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-r C SCREEN


          ==================================================
          OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:52:34



 *** 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      2.04272875E+04    2.02809885E+04    2.02809885E+04    2.59209707E-02
 V2     -2.95468613E+01   -2.92651700E+01   -2.92651700E+01    1.40177728E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.45250655E+04    2.43700032E+04    2.43700032E+04    9.62418615E-02
 V16    -8.85015065E+00   -8.56463143E+00   -8.56463143E+00    2.78844065E-01
 V17     3.16252981E+03    3.11496011E+03    3.11496011E+03    2.49147762E-01
 V19     2.20441096E+04    2.19570767E+04    2.19570767E+04    6.73748369E-01
 V20    -7.15892204E+00   -7.01163312E+00   -7.01163312E+00    1.60351724E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   8.97639645E+00 TO   1.27915999E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   7.10644438E-03


 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20427.2875080025     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.5468612774370     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21810.2046870529     ; 6000 N REF0 !
 FUNCTION V12        298.15    15.1613087031845     ; 6000 N REF0 !
 FUNCTION V15        298.15    24525.0654991989     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.85015065440329     ; 6000 N REF0 !
 FUNCTION V17        298.15    3162.52981307340     ; 6000 N REF0 !
 FUNCTION V19        298.15    22044.1096459343     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.15892204220753     ; 6000 N REF0 !



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T
```

```
 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.       10.      -1.201     -0.1201
1 W(LIQUID,B)=0.408              0.4083      2.00E-02  3.3615E-04  1.6807E-02
1 W(BCC#1,B)=0.13                0.1316      2.00E-02  1.5545E-03  7.7726E-02
2 T=1341                          1342.       10.      0.7529      7.5285E-02
2 HTR=3727                        3678.      5.00E+02  -49.47     -9.8949E-02
3 T=1049                          1047.       10.      -1.645     -0.1645
3 W(LIQUID,A)=0.27               0.2711      2.00E-02  1.1266E-03  5.6332E-02
3 W(BCC#1,A)=9.3E-2              9.5336E-02  2.00E-02  2.3361E-03  0.1168
5 T=726                           724.5       10.      -1.543     -0.1543
5 X(BCC#1,B)=3.7E-2              3.6647E-02  2.00E-02 -3.5272E-04 -1.7636E-02
5 X(BCC#2,A)=0.114               0.1147      2.00E-02  6.9816E-04  3.4908E-02
6 X(BCC#1,B)=3.7E-2              3.7082E-02  2.00E-02  8.1763E-05  4.0882E-03
6 X(BCC#2,A)=0.114               0.1158      2.00E-02  1.7838E-03  8.9192E-02
10 W(LIQUID,A)=2E-2              1.9559E-02  2.00E-02 -4.4094E-04 -2.2047E-02
11 W(LIQUID,A)=4.2E-2            4.1814E-02  2.00E-02 -1.8577E-04 -9.2885E-03
12 W(LIQUID,A)=6.5E-2            6.4837E-02  2.00E-02 -1.6291E-04 -8.1454E-03
13 W(LIQUID,A)=9.3E-2            9.2549E-02  2.00E-02 -4.5092E-04 -2.2546E-02
20 W(LIQUID,A)=0.104             0.1036      2.00E-02 -3.9164E-04 -1.9582E-02
20 W(FCC,A)=3.8E-2               3.8356E-02  2.00E-02  3.5602E-04  1.7801E-02
21 W(LIQUID,A)=0.136             0.1362      2.00E-02  1.9255E-04  9.6277E-03
21 W(FCC,A)=4.7E-2               4.7367E-02  2.00E-02  3.6734E-04  1.8367E-02
22 W(LIQUID,A)=0.187             0.1862      2.00E-02 -7.9799E-04 -3.9899E-02
22 W(FCC,A)=5.9E-2               5.9518E-02  2.00E-02  5.1760E-04  2.5880E-02
23 W(LIQUID,A)=0.245             0.2452      2.00E-02  1.8352E-04  9.1761E-03
23 W(BCC#1,A)=8.5E-2             8.6989E-02  2.00E-02  1.9894E-03  9.9469E-02


PARROT:
PARROT: @@ Note that all other experiments are well fitted.
PARROT: @@ Try to improve by optimizing a little more...
PARROT: resc
PARROT: opt 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    1.27915999E-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    1.27932257E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    1.32349424E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.27975275E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27918242E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27915986E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27919893E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27914895E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27686415E-01
  1  1.0000E+00   2  9.9998E-01   3  1.0000E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0002E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    1.27670629E-01
  1  9.9993E-01   2  9.9993E-01   3  9.9998E-01   4  1.0000E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0002E+00

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED    9 iterations
  1  9.9993E-01   2  9.9993E-01   3  9.9998E-01   4  1.0000E+00   5  1.0001E+00
  6  1.0001E+00   7  1.0002E+00
```

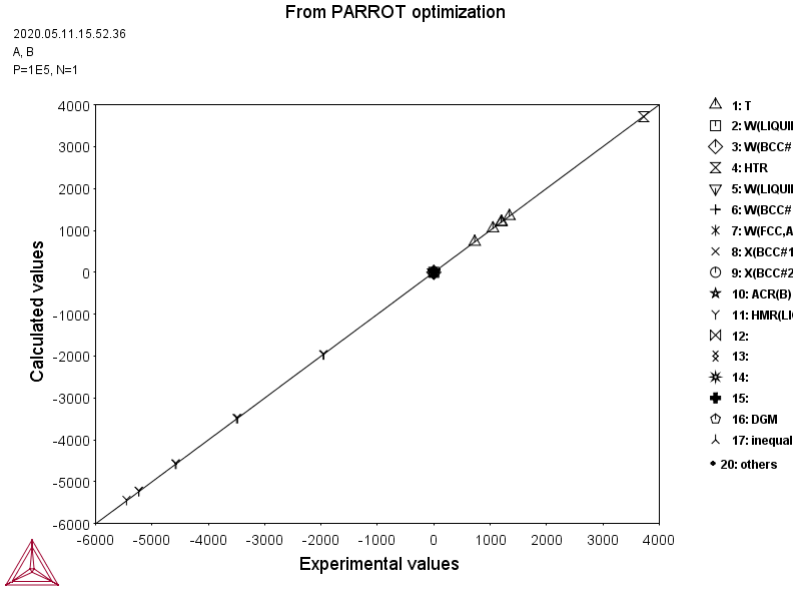
```
  1 -1.2292E-01   2  1.8762E-02   3  7.8915E-02   4  6.1120E-02   5 -9.7983E-02
  6 -1.6559E-01   7  5.7097E-02   8  1.1773E-01   9 -1.5386E-01  10 -1.7437E-02
 11  3.6109E-02  12  4.2281E-03  13  9.0250E-02  14 -2.1977E-02  15 -9.1582E-03
 16 -7.9707E-03  17 -2.2338E-02  18 -1.9366E-02  19  1.8043E-02  20  9.8524E-03
 21  1.8643E-02  22 -3.9695E-02  23  2.6185E-02  24  9.6601E-03  25  1.0017E-01

              THE SUM OF SQUARES IS   1.27670629E-01
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:52:34



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  10


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04258378E+04    2.04272875E+04    2.04272875E+04    2.56056982E-02
 V2     -2.95449125E+01   -2.95468613E+01   -2.95468613E+01    1.38446586E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.45244729E+04    2.45250655E+04    2.45250655E+04    9.63618809E-02
 V16    -8.85034455E+00   -8.85015065E+00   -8.85015065E+00    2.70402373E-01
 V17     3.16285524E+03    3.16252981E+03    3.16252981E+03    2.49505588E-01
 V19     2.20452445E+04    2.20441096E+04    2.20441096E+04    6.66480578E-01
 V20    -7.16035823E+00   -7.15892204E+00   -7.15892204E+00    1.56211863E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.27915999E-01 TO   1.27670629E-01
 DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   7.09281270E-03


 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20425.8378295492     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.5449125489583     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21810.2046870529     ; 6000 N REF0 !
 FUNCTION V12        298.15    15.1613087031845     ; 6000 N REF0 !
 FUNCTION V15        298.15    24524.4729175200     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.85034455335361     ; 6000 N REF0 !
 FUNCTION V17        298.15    3162.85523540043     ; 6000 N REF0 !
 FUNCTION V19        298.15    22045.2444507111     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.16035822781115     ; 6000 N REF0 !



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.       10.      -1.229     -0.1229
```

```
1 W(LIQUID,B)=0.408              0.4084      2.00E-02  3.7523E-04  1.8762E-02
1 W(BCC#1,B)=0.13                0.1316      2.00E-02  1.5783E-03  7.8915E-02
2 T=1341                          1342.       10.      0.6112      6.1120E-02
2 HTR=3727                        3678.      5.00E+02  -48.99     -9.7983E-02
3 T=1049                          1047.       10.      -1.656     -0.1656
3 W(LIQUID,A)=0.27               0.2711      2.00E-02  1.1419E-03  5.7097E-02
3 W(BCC#1,A)=9.3E-2              9.5355E-02  2.00E-02  2.3545E-03  0.1177
5 T=726                           724.5       10.      -1.539     -0.1539
5 X(BCC#1,B)=3.7E-2              3.6651E-02  2.00E-02 -3.4874E-04 -1.7437E-02
5 X(BCC#2,A)=0.114               0.1147      2.00E-02  7.2219E-04  3.6109E-02
6 X(BCC#1,B)=3.7E-2              3.7085E-02  2.00E-02  8.4562E-05  4.2281E-03
6 X(BCC#2,A)=0.114               0.1158      2.00E-02  1.8050E-03  9.0250E-02
10 W(LIQUID,A)=2E-2              1.9560E-02  2.00E-02 -4.3955E-04 -2.1977E-02
11 W(LIQUID,A)=4.2E-2            4.1817E-02  2.00E-02 -1.8316E-04 -9.1582E-03
12 W(LIQUID,A)=6.5E-2            6.4841E-02  2.00E-02 -1.5941E-04 -7.9707E-03
13 W(LIQUID,A)=9.3E-2            9.2553E-02  2.00E-02 -4.4677E-04 -2.2338E-02
20 W(LIQUID,A)=0.104             0.1036      2.00E-02 -3.8733E-04 -1.9366E-02
20 W(FCC,A)=3.8E-2               3.8361E-02  2.00E-02  3.6086E-04  1.8043E-02
21 W(LIQUID,A)=0.136             0.1362      2.00E-02  1.9705E-04  9.8524E-03
21 W(FCC,A)=4.7E-2               4.7373E-02  2.00E-02  3.7286E-04  1.8643E-02
22 W(LIQUID,A)=0.187             0.1862      2.00E-02 -7.9389E-04 -3.9695E-02
22 W(FCC,A)=5.9E-2               5.9524E-02  2.00E-02  5.2371E-04  2.6185E-02
23 W(LIQUID,A)=0.245             0.2452      2.00E-02  1.9320E-04  9.6601E-03
23 W(BCC#1,A)=8.5E-2             8.7003E-02  2.00E-02  2.0035E-03  0.1002


PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram again
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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:   6.813E-01  7.245E+02
 ** A2B
    BCC#1
 ** BCC#2

Phase region boundary   4 at:   3.620E-01  7.245E+02
 ** A2B
    BCC#1
Calculated.                      15 equilibria

Phase region boundary   5 at:   3.775E-01  1.192E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.837E-01  1.192E+03
 ** LIQUID
    BCC#1
Calculated                      26 equilibria

Phase region boundary   7 at:   4.865E-01  1.192E+03
 ** LIQUID
    A2B
Calculated.                      33 equilibria

Phase region boundary   8 at:   6.495E-01  1.047E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.626E-01  1.047E+03
    A2B
 ** BCC#1
Calculated.                      11 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.258E-01  1.047E+03
    LIQUID
 ** BCC#1
Calculated.                       9 equilibria

Phase region boundary  11 at:   8.763E-01  1.212E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.820E-01  1.212E+03
    LIQUID
 ** FCC
Calculated                      31 equilibria

Phase region boundary  13 at:   9.355E-01  1.212E+03
    BCC#1
 ** FCC
Calculated                      23 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
```

```
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   3.642E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                      10 equilibria

Phase region boundary  26 at:   3.642E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   3.642E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  28 at:   7.905E-01  7.700E+02
 ** A2B
    BCC#1
Calculated                      10 equilibria

Phase region boundary  29 at:   7.905E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:   7.905E-01  7.700E+02
 ** A2B
    BCC#1
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   2.451E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:   2.451E-01  1.230E+03
 ** LIQUID
    BCC#1
Calculated                      26 equilibria

Phase region boundary  33 at:   8.859E-01  1.230E+03
 ** LIQUID
    FCC
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary  34 at:   8.859E-01  1.230E+03
 ** LIQUID
    FCC
Calculated                      29 equilibria

Phase region boundary  35 at:   6.428E-03  1.397E+03
    LIQUID
 ** BCC#1
Calculated                      9 equilibria

Phase region boundary  36 at:   6.428E-03  1.397E+03
    LIQUID
 ** BCC#1
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  37 at:   2.303E-01  1.244E+03
    LIQUID
 ** BCC#1
Calculated                      21 equilibria

Phase region boundary  38 at:   2.303E-01  1.244E+03
    LIQUID
 ** BCC#1
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  39 at:   6.122E-01  1.239E+03
    LIQUID
 ** A2B
Calculated.                      14 equilibria
Terminating at known equilibrium

Phase region boundary  40 at:   6.122E-01  1.239E+03
    LIQUID
 ** A2B
Calculated.                      8 equilibria
Terminating at known equilibrium

Phase region boundary  41 at:   9.927E-01  1.613E+03
```

```
     LIQUID
  ** FCC
 Calculated.                      19 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      10 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     1 seconds
POLY: post
POST: s-l d
POST: plot
```




```
POST:
POST: set-inter
POST:Hit RETURN to continue
POST: ba
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid
PARROT: @@ at high B. Restore equilibrium 4 on the POP file
PARROT: ed
ED_EXP: read 1
ED_EXP: s-e 4
 Equilibrium number                     4, label AINV
ED_EXP: s-we 1
Equilibria (range) or label(s) /PRESENT/: PRESENT
ED_EXP: s-a-s
T /1204.179215/: 1200
Automatic start values for phase constituents? /N/: N

 Phase LIQUID
Major constituent(s) /b/: b

 Phase BCC
Major constituent(s) /b/: b

 Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
 Testing result with global minimization
    13 ITS,  CPU TIME USED   0 SECONDS
ED_EXP: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     4, label AINV, database:

 Conditions:
 P=1.01325E5
 FIXED PHASES
 LIQUID=1  BCC#1=1   FCC=1
 DEGREES OF FREEDOM 0

 Temperature   1211.86 K (   938.71 C),  Pressure  1.013250E+05
 Number of moles of components  3.00000E+00,  Mass in grams  1.30242E+02
 Total Gibbs energy -1.00423E+04,  Enthalpy  1.99596E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.5861E-01  1.0114E-01 3.8286E-01 -9.6738E+03 SER
 B                       2.3414E+00  8.9886E-01 8.5590E-01 -1.5679E+03 SER

 FCC                        Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5895E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.40376E-01  A  5.96239E-02

 BCC#1                      Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.5283E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  9.30557E-01  A  6.94426E-02

 LIQUID                     Status FIXED       Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 3.9063E+01, Volume fraction 0.0000E+00  Mass fractions:
 B  8.13351E-01  A  1.86649E-01
 EXPERIMENT T=1203:DT  $1211.86:10  NO=1
 EXPERIMENT W(LIQUID,A)=0.19:DX  $0.186649:2E-2  NO=2
 EXPERIMENT W(BCC#1,A)=6.9E-2:DX  $6.94426E-2:2E-2  NO=3
 EXPERIMENT W(FCC,A)=6E-2:DX  $5.96239E-2:2E-2  NO=4
```

```
ED_EXP: @@ Now equilibrium 4 is on the high B side
ED_EXP: save
ED_EXP: ba
PARROT: resc
PARROT: opt 0
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:52:58



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:   0


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =   0   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04258378E+04    2.04258378E+04    2.04258378E+04    0.00000000E+00
 V2     -2.95449125E+01   -2.95449125E+01   -2.95449125E+01    0.00000000E+00
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.45244729E+04    2.45244729E+04    2.45244729E+04    0.00000000E+00
 V16    -8.85034455E+00   -8.85034455E+00   -8.85034455E+00    0.00000000E+00
 V17     3.16285524E+03    3.16285524E+03    3.16285524E+03    0.00000000E+00
 V19     2.20452445E+04    2.20452445E+04    2.20452445E+04    0.00000000E+00
 V20    -7.16035823E+00   -7.16035823E+00   -7.16035823E+00    0.00000000E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   0.00000000E+00 TO   9.41736782E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   4.28062174E-02


 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20425.8378295492     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.5449125489583     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21810.2046870529     ; 6000 N REF0 !
 FUNCTION V12        298.15    15.1613087031845     ; 6000 N REF0 !
 FUNCTION V15        298.15    24524.4729175200     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.85034455335361     ; 6000 N REF0 !
 FUNCTION V17        298.15    3162.85523540043     ; 6000 N REF0 !
 FUNCTION V19        298.15    22045.2444507111     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.16035822781115     ; 6000 N REF0 !



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T


$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.       10.      -1.229     -0.1229
1 W(LIQUID,B)=0.408              0.4084      2.00E-02  3.7523E-04  1.8762E-02
```

```
1 W(BCC#1,B)=0.13                0.1316      2.00E-02  1.5783E-03  7.8915E-02
2 T=1341                          1342.       10.      0.6112      6.1120E-02
2 HTR=3727                        3678.      5.00E+02  -48.99     -9.7983E-02
3 T=1049                          1047.       10.      -1.656     -0.1656
3 W(LIQUID,A)=0.27               0.2711      2.00E-02  1.1419E-03  5.7097E-02
3 W(BCC#1,A)=9.3E-2              9.5355E-02  2.00E-02  2.3545E-03  0.1177
4 T=1203                          1212.       10.       8.861      0.8861
4 W(LIQUID,A)=0.19               0.1866      2.00E-02 -3.3513E-03 -0.1676
4 W(BCC#1,A)=6.9E-2              6.9443E-02  2.00E-02  4.4257E-04  2.2128E-02
4 W(FCC,A)=6E-2                  5.9624E-02  2.00E-02 -3.7607E-04 -1.8803E-02
5 T=726                           724.5       10.      -1.539     -0.1539
5 X(BCC#1,B)=3.7E-2              3.6651E-02  2.00E-02 -3.4874E-04 -1.7437E-02
5 X(BCC#2,A)=0.114               0.1147      2.00E-02  7.2219E-04  3.6109E-02
6 X(BCC#1,B)=3.7E-2              3.7085E-02  2.00E-02  8.4562E-05  4.2281E-03
6 X(BCC#2,A)=0.114               0.1158      2.00E-02  1.8050E-03  9.0250E-02
10 W(LIQUID,A)=2E-2              1.9560E-02  2.00E-02 -4.3955E-04 -2.1977E-02
11 W(LIQUID,A)=4.2E-2            4.1817E-02  2.00E-02 -1.8316E-04 -9.1582E-03
12 W(LIQUID,A)=6.5E-2            6.4841E-02  2.00E-02 -1.5941E-04 -7.9707E-03
13 W(LIQUID,A)=9.3E-2            9.2553E-02  2.00E-02 -4.4677E-04 -2.2338E-02
20 W(LIQUID,A)=0.104             0.1036      2.00E-02 -3.8733E-04 -1.9366E-02
20 W(FCC,A)=3.8E-2               3.8361E-02  2.00E-02  3.6086E-04  1.8043E-02
21 W(LIQUID,A)=0.136             0.1362      2.00E-02  1.9705E-04  9.8524E-03
21 W(FCC,A)=4.7E-2               4.7373E-02  2.00E-02  3.7286E-04  1.8643E-02
22 W(LIQUID,A)=0.187             0.1862      2.00E-02 -7.9389E-04 -3.9695E-02
22 W(FCC,A)=5.9E-2               5.9524E-02  2.00E-02  5.2371E-04  2.6185E-02
23 W(LIQUID,A)=0.245             0.2452      2.00E-02  1.9320E-04  9.6601E-03
23 W(BCC#1,A)=8.5E-2             8.7003E-02  2.00E-02  2.0035E-03  0.1002


PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 30
 Use      29 experiments, maximum is        2000
 Use     554 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A


      AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    9.41736782E-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    9.42554355E-01
  1  1.0001E+00   2  1.0000E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    9.44643539E-01
  1  1.0000E+00   2  1.0001E+00   3  1.0000E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    9.18434396E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    9.28575122E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0001E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    9.20480305E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0001E+00
  6  1.0000E+00   7  1.0000E+00

      AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    9.35681019E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0001E+00   7  1.0000E+00

      AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    9.11696487E-01
  1  1.0000E+00   2  1.0000E+00   3  1.0001E+00   4  1.0000E+00   5  1.0000E+00
  6  1.0000E+00   7  1.0001E+00

      AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    2.18168196E-01
  1  1.0000E+00   2  9.9999E-01   3  1.0034E+00   4  9.9857E-01   5  9.9971E-01
  6  9.9757E-01   7  1.0011E+00

      AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    2.07235077E-01
  1  9.9990E-01   2  1.0000E+00   3  1.0024E+00   4  9.9680E-01   5  9.9848E-01
  6  9.9610E-01   7  9.9760E-01

      AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    1.87994114E-01
  1  9.9973E-01   2  9.9985E-01   3  1.0004E+00   4  9.9280E-01   5  9.9574E-01
  6  9.9339E-01   7  9.9099E-01

      AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.62151848E-01
  1  9.9932E-01   2  9.9968E-01   3  9.9655E-01   4  9.8495E-01   5  9.9036E-01
  6  9.8792E-01   7  9.7763E-01

      AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.50053566E-01
  1  9.9877E-01   2  9.9938E-01   3  9.9141E-01   4  9.7448E-01   5  9.8315E-01
  6  9.8103E-01   7  9.6066E-01

     THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   12 iterations
  1  9.9877E-01   2  9.9938E-01   3  9.9141E-01   4  9.7448E-01   5  9.8315E-01
  6  9.8103E-01   7  9.6066E-01

  1 -1.1651E-01   2  1.0617E-02   3  6.2552E-02   4  6.6364E-02   5 -8.1216E-02
  6 -2.1958E-01   7  4.1235E-02   8  8.3058E-02   9  2.9863E-02  10  2.5417E-02
 11  4.5304E-02  12  5.9829E-02  13 -1.7379E-01  14  1.8247E-02  15  4.5330E-02
 16  4.3059E-02  17  1.0640E-01  18 -2.3843E-02  19 -1.1306E-02  20 -8.6872E-03
 21 -1.9428E-02  22 -1.4518E-02  23  2.3484E-02  24  2.1765E-02  25  3.3281E-02
 26 -1.3748E-02  27  6.4932E-02  28 -2.4111E-02  29  5.6807E-02

                THE SUM OF SQUARES IS   1.50053566E-01
PARROT: l-r C SCREEN


            ==================================================
            OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:52:58



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  13


 == OPTIMIZING CONDITIONS ==
```

```
  RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
  MINIMUM SAVE ON FILE: Y
  ERROR FOR INEQUALITIES =  1.00000000E+00
  RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
  MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
  ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1  TO V00

VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
V1      2.04006875E+04    2.04258378E+04    2.04258378E+04    2.41616565E-02
V2     -2.95264884E+01   -2.95449125E+01   -2.95449125E+01    1.31557074E-02
V11    -2.18102047E+04
V12     1.51613087E+01
V15     2.43137486E+04    2.45244729E+04    2.45244729E+04    7.66766115E-02
V16    -8.62447822E+00   -8.85034455E+00   -8.85034455E+00    2.08107833E-01
V17     3.10957096E+03    3.16285524E+03    3.16285524E+03    2.22191978E-01
V19     2.16271391E+04    2.20452445E+04    2.20452445E+04    4.98933492E-01
V20    -6.87864890E+00   -7.16035823E+00   -7.16035823E+00    1.22727292E+00

NUMBER OF OPTIMIZING VARIABLES :   7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM   9.41736782E-01 TO   1.50053566E-01
DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   6.82061665E-03


SYMBOL        STATUS   VALUE/FUNCTION
FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
  2 RTLNP     20000000 +R*T*LN(1E-05*P)
FUNCTION V1         298.15    20400.6875006067     ; 6000 N REF0 !
FUNCTION V2         298.15   -29.5264883725907     ; 6000 N REF0 !
FUNCTION V11        298.15   -21810.2046870529     ; 6000 N REF0 !
FUNCTION V12        298.15    15.1613087031845     ; 6000 N REF0 !
FUNCTION V15        298.15    24313.7485780243     ; 6000 N REF0 !
FUNCTION V16        298.15   -8.62447822190065     ; 6000 N REF0 !
FUNCTION V17        298.15    3109.57096384564     ; 6000 N REF0 !
FUNCTION V19        298.15    21627.1391048280     ; 6000 N REF0 !
FUNCTION V20        298.15   -6.87864889801350     ; 6000 N REF0 !



LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
   CONSTITUENTS: A,B

     G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
     G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
     L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
     L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


A2B
 2 SUBLATTICES, SITES  2:  1
   CONSTITUENTS: A : B

     G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
            500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


BCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
   CONSTITUENTS: A,B

     G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
     G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
     L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
     L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


FCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
   CONSTITUENTS: A,B

     G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
     G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
     L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
     L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.       10.      -1.165     -0.1165
1 W(LIQUID,B)=0.408              0.4082      2.00E-02  2.1234E-04  1.0617E-02
1 W(BCC#1,B)=0.13                0.1313      2.00E-02  1.2510E-03  6.2552E-02
2 T=1341                          1342.       10.      0.6636      6.6364E-02
2 HTR=3727                        3686.      5.00E+02  -40.61     -8.1216E-02
3 T=1049                          1047.       10.      -2.196     -0.2196
3 W(LIQUID,A)=0.27               0.2708      2.00E-02  8.2469E-04  4.1235E-02
3 W(BCC#1,A)=9.3E-2              9.4661E-02  2.00E-02  1.6612E-03  8.3058E-02
4 T=1203                          1203.       10.      0.2986      2.9863E-02
4 W(LIQUID,A)=0.19               0.1905      2.00E-02  5.0833E-04  2.5417E-02
4 W(BCC#1,A)=6.9E-2              6.9906E-02  2.00E-02  9.0608E-04  4.5304E-02
4 W(FCC,A)=6E-2                  6.1197E-02  2.00E-02  1.1966E-03  5.9829E-02
5 T=726                           724.3       10.      -1.738     -0.1738
5 X(BCC#1,B)=3.7E-2              3.7365E-02  2.00E-02  3.6493E-04  1.8247E-02
5 X(BCC#2,A)=0.114               0.1149      2.00E-02  9.0661E-04  4.5330E-02
6 X(BCC#1,B)=3.7E-2              3.7861E-02  2.00E-02  8.6118E-04  4.3059E-02
6 X(BCC#2,A)=0.114               0.1161      2.00E-02  2.1279E-03  0.1064
10 W(LIQUID,A)=2E-2              1.9523E-02  2.00E-02 -4.7686E-04 -2.3843E-02
11 W(LIQUID,A)=4.2E-2            4.1774E-02  2.00E-02 -2.2612E-04 -1.1306E-02
12 W(LIQUID,A)=6.5E-2            6.4826E-02  2.00E-02 -1.7374E-04 -8.6872E-03
13 W(LIQUID,A)=9.3E-2            9.2611E-02  2.00E-02 -3.8856E-04 -1.9428E-02
20 W(LIQUID,A)=0.104             0.1037      2.00E-02 -2.9035E-04 -1.4518E-02
20 W(FCC,A)=3.8E-2               3.8470E-02  2.00E-02  4.6968E-04  2.3484E-02
21 W(LIQUID,A)=0.136             0.1364      2.00E-02  4.3530E-04  2.1765E-02
```

```
21 W(FCC,A)=4.7E-2                4.7666E-02  2.00E-02  6.6563E-04  3.3281E-02
22 W(LIQUID,A)=0.187              0.1867      2.00E-02 -2.7497E-04 -1.3748E-02
22 W(FCC,A)=5.9E-2                6.0299E-02  2.00E-02  1.2986E-03  6.4932E-02
23 W(LIQUID,A)=0.245              0.2445      2.00E-02 -4.8222E-04 -2.4111E-02
23 W(BCC#1,A)=8.5E-2              8.6136E-02  2.00E-02  1.1361E-03  5.6807E-02


PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Now optimize all parameters and all experiments
PARROT: l-a-v
OUTPUT TO SCREEN OR FILE /SCREEN/:

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.04006875E+04    2.04258378E+04    2.04258378E+04    2.41616565E-02
 V2     -2.95264884E+01   -2.95449125E+01   -2.95449125E+01    1.31557074E-02
 V11    -2.18102047E+04
 V12     1.51613087E+01
 V15     2.43137486E+04    2.45244729E+04    2.45244729E+04    7.66766115E-02
 V16    -8.62447822E+00   -8.85034455E+00   -8.85034455E+00    2.08107833E-01
 V17     3.10957096E+03    3.16285524E+03    3.16285524E+03    2.22191978E-01
 V19     2.16271391E+04    2.20452445E+04    2.20452445E+04    4.98933492E-01
 V20    -6.87864890E+00   -7.16035823E+00   -7.16035823E+00    1.22727292E+00

 NUMBER OF OPTIMIZING VARIABLES :   7
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   9.41736782E-01 TO   1.50053566E-01
 DEGREES OF FREEDOM   22.  REDUCED SUM OF SQUARES   6.82061665E-03
PARROT: s-o-v 11-12
PARROT: ed
ED_EXP: read 1
ED_EXP: c-a
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1191.8      LIQUID A2B BCC
   2 AINV   2   1.    1341.7      LIQUID A2B
   3 AINV   2   1.    1046.8      LIQUID A2B BCC
   4 AINV   2   1.    1203.3      LIQUID BCC FCC
   5 AINV   2   1.     724.3      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    2   1.    1594.0      LIQUID FCC
  11 ALF    2   1.    1548.0      LIQUID FCC
  12 ALF    2   1.    1499.0      LIQUID FCC
  13 ALF    2   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA   < unused >  1573.0      LIQUID
 101 AA   < unused >  1573.0      LIQUID
 102 AA   < unused >  1573.0      LIQUID
 103 AA   < unused >  1573.0      LIQUID
 104 AA   < unused >  1573.0      LIQUID
 105 AA   < unused >  1573.0      LIQUID
 106 AA   < unused >  1573.0      LIQUID
 107 AA   < unused >  1573.0      LIQUID
 108 AA   < unused >  1573.0      LIQUID
 110 AH   < unused >  1773.0      LIQUID
 111 AH   < unused >  1773.0      LIQUID
 112 AH   < unused >  1773.0      LIQUID
 113 AH   < unused >  1773.0      LIQUID
 114 AH   < unused >  1773.0      LIQUID
 115 AH   < unused >  1773.0      LIQUID
 116 AH   < unused >  1773.0      LIQUID
 117 AH   < unused >  1773.0      LIQUID
 118 AH   < unused >  1773.0      LIQUID
ED_EXP: s-we 1 100-118
ED_EXP: s-e 1
 Equilibrium number                      1, label AINV
ED_EXP: c-a
 Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
   1 AINV   2   1.    1191.8      LIQUID A2B BCC
   2 AINV   2   1.    1341.7      LIQUID A2B
   3 AINV   2   1.    1046.8      LIQUID A2B BCC
   4 AINV   2   1.    1203.3      LIQUID BCC FCC
   5 AINV   2   1.     724.3      A2B BCC BCC#2
   6 AINV   2   1.     726.0      BCC BCC#2
  10 ALF    2   1.    1594.0      LIQUID FCC
  11 ALF    2   1.    1548.0      LIQUID FCC
  12 ALF    2   1.    1499.0      LIQUID FCC
  13 ALF    2   1.    1438.0      LIQUID FCC
  20 ATIE   2   1.    1413.0      LIQUID FCC
  21 ATIE   2   1.    1337.0      LIQUID FCC
  22 ATIE   2   1.    1213.0      LIQUID FCC
  23 ATIE   2   1.    1100.0      LIQUID BCC
 100 AA     2   1.    1573.0      LIQUID
 101 AA     2   1.    1573.0      LIQUID
 102 AA     2   1.    1573.0      LIQUID
 103 AA     2   1.    1573.0      LIQUID
 104 AA     2   1.    1573.0      LIQUID
 105 AA     2   1.    1573.0      LIQUID
 106 AA     2   1.    1573.0      LIQUID
 107 AA     2   1.    1573.0      LIQUID
 108 AA     2   1.    1573.0      LIQUID
 110 AH     2   1.    1773.0      LIQUID
 111 AH     2   1.    1773.0      LIQUID
 112 AH     2   1.    1773.0      LIQUID
 113 AH     2   1.    1773.0      LIQUID
 114 AH     2   1.    1773.0      LIQUID
 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
ED_EXP: ba
PARROT: opt 30
 Use      47 experiments, maximum is        2000
 Use    1082 real workspace, maximum is    50000
    The following output is provided by subroutine VA05A
```

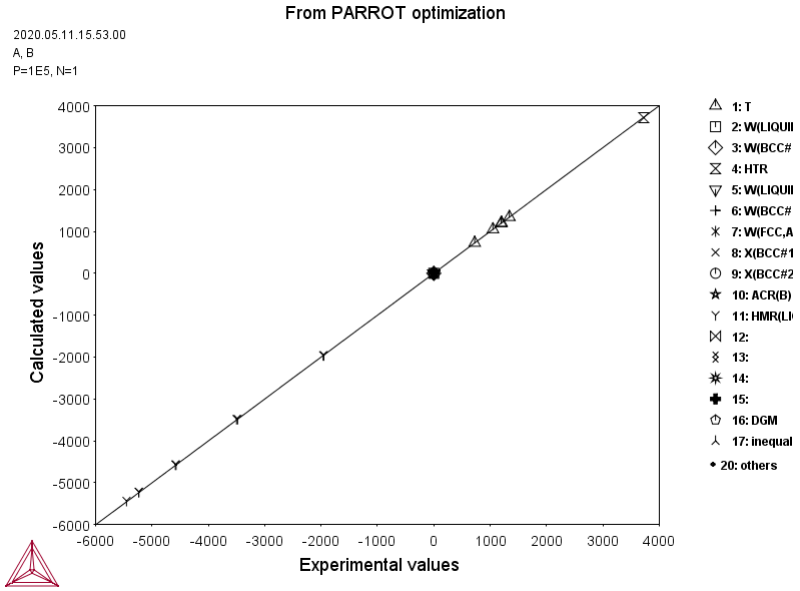
```
     AT THE    0 TH ITERATION WE HAVE THE SUM OF SQUARES    1.71348979E-01
 1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0000E+00   5  9.9141E-01
 6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

     AT THE    1 ST ITERATION WE HAVE THE SUM OF SQUARES    1.72203926E-01
 1  9.9887E-01   2  9.9938E-01   3  1.0000E+00   4  1.0000E+00   5  9.9141E-01
 6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

     AT THE    2 ND ITERATION WE HAVE THE SUM OF SQUARES    1.74167080E-01
 1  9.9877E-01   2  9.9948E-01   3  1.0000E+00   4  1.0000E+00   5  9.9141E-01
 6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

     AT THE    3 RD ITERATION WE HAVE THE SUM OF SQUARES    1.75634352E-01
 1  9.9877E-01   2  9.9938E-01   3  1.0001E+00   4  1.0000E+00   5  9.9141E-01
 6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

     AT THE    4 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69474648E-01
 1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
 6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

     AT THE    5 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69562794E-01
 1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9151E-01
 6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

     AT THE    6 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69566263E-01
 1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
 6  9.7458E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

     AT THE    7 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69484796E-01
 1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
 6  9.7448E-01   7  9.8325E-01   8  9.8103E-01   9  9.6066E-01

     AT THE    8 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69600690E-01
 1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
 6  9.7448E-01   7  9.8315E-01   8  9.8113E-01   9  9.6066E-01

     AT THE    9 TH ITERATION WE HAVE THE SUM OF SQUARES    1.69486722E-01
 1  9.9877E-01   2  9.9938E-01   3  1.0000E+00   4  1.0001E+00   5  9.9141E-01
 6  9.7448E-01   7  9.8315E-01   8  9.8103E-01   9  9.6076E-01

     AT THE   10 TH ITERATION WE HAVE THE SUM OF SQUARES    1.52786178E-01
 1  9.9900E-01   2  9.9895E-01   3  9.9938E-01   4  1.0004E+00   5  9.9144E-01
 6  9.7447E-01   7  9.8315E-01   8  9.8103E-01   9  9.6066E-01

     AT THE   11 TH ITERATION WE HAVE THE SUM OF SQUARES    1.40532741E-01
 1  9.9890E-01   2  9.9900E-01   3  9.9926E-01   4  1.0005E+00   5  9.9136E-01
 6  9.7393E-01   7  9.8302E-01   8  9.8140E-01   9  9.6114E-01

     AT THE   12 TH ITERATION WE HAVE THE SUM OF SQUARES    1.29724491E-01
 1  9.9893E-01   2  9.9866E-01   3  9.9885E-01   4  1.0007E+00   5  9.9142E-01
 6  9.7290E-01   7  9.8276E-01   8  9.8209E-01   9  9.6210E-01

     AT THE   13 TH ITERATION WE HAVE THE SUM OF SQUARES    1.15934438E-01
 1  9.9874E-01   2  9.9848E-01   3  9.9859E-01   4  1.0010E+00   5  9.9102E-01
 6  9.7065E-01   7  9.8221E-01   8  9.8360E-01   9  9.6396E-01

     AT THE   14 TH ITERATION WE HAVE THE SUM OF SQUARES    9.75379543E-02
 1  9.9849E-01   2  9.9788E-01   3  9.9801E-01   4  1.0015E+00   5  9.9032E-01
 6  9.6628E-01   7  9.8112E-01   8  9.8668E-01   9  9.6777E-01

     AT THE   15 TH ITERATION WE HAVE THE SUM OF SQUARES    7.50720965E-02
 1  9.9786E-01   2  9.9702E-01   3  9.9725E-01   4  1.0024E+00   5  9.8867E-01
 6  9.5729E-01   7  9.7889E-01   8  9.9265E-01   9  9.7533E-01

     AT THE   16 TH ITERATION WE HAVE THE SUM OF SQUARES    6.73903735E-02
 1  9.9721E-01   2  9.9606E-01   3  9.9646E-01   4  1.0033E+00   5  9.8691E-01
 6  9.4769E-01   7  9.7652E-01   8  9.9896E-01   9  9.8321E-01

    THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED   16 iterations
 1  9.9721E-01   2  9.9606E-01   3  9.9646E-01   4  1.0033E+00   5  9.8691E-01
 6  9.4769E-01   7  9.7652E-01   8  9.9896E-01   9  9.8321E-01

 1 -5.7769E-02   2 -9.3761E-03   3  1.4158E-02   4  2.0690E-02   5 -2.5688E-02
 6 -5.1171E-02   7  1.9343E-02   8  2.7056E-02   9  1.2439E-02  10  2.7688E-02
11  9.1632E-03  12  1.3813E-02  13 -4.8791E-02  14  2.1460E-02  15  4.7007E-03
16  2.8358E-02  17  2.1568E-02  18 -2.2454E-02  19 -8.9460E-03  20 -5.8150E-03
21 -1.6458E-02  22 -1.1654E-02  23  1.4345E-02  24  2.3824E-02  25  1.4109E-02
26 -1.4553E-02  27  2.0708E-02  28 -1.2425E-02  29  1.5727E-02  30 -9.5825E-03
31 -1.6802E-02  32  2.7496E-02  33  8.7112E-02  34  1.2446E-01  35  1.0182E-01
36 -1.7174E-02  37  7.0704E-02  38 -1.9397E-02  39  1.6052E-02  40  4.5425E-02
41  4.8120E-02  42  4.6137E-02  43  4.1476E-02  44  3.4137E-02  45  2.2120E-02
46  7.4249E-03  47 -1.1948E-02

               THE SUM OF SQUARES IS   6.73903735E-02
PARROT: l-r C SCREEN


           ==================================================
           OUTPUT FROM  P A R R O T.  DATE 2020. 5.11   15:52:58



 *** SUCCESSFUL OPTIMIZATION. ***
     NUMBER OF ITERATIONS:  17


 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
   MINIMUM SAVE ON FILE: Y
   ERROR FOR INEQUALITIES =  1.00000000E+00
   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04
 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
   MAXFUN =  30   DMAX =  1.00000000E+02   H =  1.00000000E-04
   ACC = (INITIAL SUM OF SQUARES) *  1.00000000E-03



 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE              START VALUE       SCALING FACTOR    REL.STAND.DEV
 V1      2.03688341E+04    2.04258378E+04    2.04258378E+04    2.96135416E-02
```

```
 V2     -2.94286301E+01   -2.95449125E+01   -2.95449125E+01    2.25274567E-02
 V11    -2.17330472E+04   -2.18102047E+04   -2.18102047E+04    3.47407502E-02
 V12     1.52107324E+01    1.51613087E+01    1.51613087E+01    5.56505566E-02
 V15     2.42035190E+04    2.45244729E+04    2.45244729E+04    8.09093797E-02
 V16    -8.38741946E+00   -8.85034455E+00   -8.85034455E+00    2.37193888E-01
 V17     3.08858371E+03    3.16285524E+03    3.16285524E+03    2.23457303E-01
 V19     2.20222843E+04    2.20452445E+04    2.20452445E+04    4.94492771E-01
 V20    -7.04010396E+00   -7.16035823E+00   -7.16035823E+00    1.21662443E+00

 NUMBER OF OPTIMIZING VARIABLES :   9
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   1.71348979E-01 TO   6.73903735E-02
 DEGREES OF FREEDOM   38.  REDUCED SUM OF SQUARES   1.77343088E-03


 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 FUNCTION V1         298.15    20368.8340877061     ; 6000 N REF0 !
 FUNCTION V2         298.15   -29.4286300929314     ; 6000 N REF0 !
 FUNCTION V11        298.15   -21733.0471557439     ; 6000 N REF0 !
 FUNCTION V12        298.15    15.2107324040927     ; 6000 N REF0 !
 FUNCTION V15        298.15    24203.5190359491     ; 6000 N REF0 !
 FUNCTION V16        298.15   -8.38741946075743     ; 6000 N REF0 !
 FUNCTION V17        298.15    3088.58370732035     ; 6000 N REF0 !
 FUNCTION V19        298.15    22022.2842727268     ; 6000 N REF0 !
 FUNCTION V20        298.15   -7.04010395678532     ; 6000 N REF0 !



 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T
      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T
      L(LIQUID,A,B;1) =    500.00<T< 2000.00: +V13+V14*T


 A2B
  2 SUBLATTICES, SITES  2:  1
    CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)


 BCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +0.0
      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +0.0
      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T


 FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +408
      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T



$ ======  BLOCK NUMBER  1

 DEFINED CONSTANTS
    DX=2E-2, P0=101325, DH=500, DT=10
 DEFINED FUNCTIONS AND VARIABLES%
    HTR=HM(LIQUID)-HM(A2B)
1 T=1193                          1192.       10.     -0.5777     -5.7769E-02
1 W(LIQUID,B)=0.408              0.4078      2.00E-02 -1.8752E-04 -9.3761E-03
1 W(BCC#1,B)=0.13                0.1303      2.00E-02  2.8316E-04  1.4158E-02
2 T=1341                          1341.       10.      0.2069      2.0690E-02
2 HTR=3727                        3714.      5.00E+02  -12.84     -2.5688E-02
3 T=1049                          1048.       10.     -0.5117     -5.1171E-02
3 W(LIQUID,A)=0.27               0.2704      2.00E-02  3.8687E-04  1.9343E-02
3 W(BCC#1,A)=9.3E-2              9.3541E-02  2.00E-02  5.4112E-04  2.7056E-02
4 T=1203                          1203.       10.      0.1244      1.2439E-02
4 W(LIQUID,A)=0.19               0.1906      2.00E-02  5.5376E-04  2.7688E-02
4 W(BCC#1,A)=6.9E-2              6.9183E-02  2.00E-02  1.8326E-04  9.1632E-03
4 W(FCC,A)=6E-2                  6.0276E-02  2.00E-02  2.7626E-04  1.3813E-02
5 T=726                           725.5       10.     -0.4879     -4.8791E-02
5 X(BCC#1,B)=3.7E-2              3.7429E-02  2.00E-02  4.2920E-04  2.1460E-02
5 X(BCC#2,A)=0.114               0.1141      2.00E-02  9.4014E-05  4.7007E-03
6 X(BCC#1,B)=3.7E-2              3.7567E-02  2.00E-02  5.6715E-04  2.8358E-02
6 X(BCC#2,A)=0.114               0.1144      2.00E-02  4.3136E-04  2.1568E-02
10 W(LIQUID,A)=2E-2              1.9551E-02  2.00E-02 -4.4908E-04 -2.2454E-02
11 W(LIQUID,A)=4.2E-2            4.1821E-02  2.00E-02 -1.7892E-04 -8.9460E-03
12 W(LIQUID,A)=6.5E-2            6.4884E-02  2.00E-02 -1.1630E-04 -5.8150E-03
13 W(LIQUID,A)=9.3E-2            9.2671E-02  2.00E-02 -3.2917E-04 -1.6458E-02
20 W(LIQUID,A)=0.104             0.1038      2.00E-02 -2.3309E-04 -1.1654E-02
20 W(FCC,A)=3.8E-2               3.8287E-02  2.00E-02  2.8690E-04  1.4345E-02
21 W(LIQUID,A)=0.136             0.1365      2.00E-02  4.7648E-04  2.3824E-02
21 W(FCC,A)=4.7E-2               4.7282E-02  2.00E-02  2.8217E-04  1.4109E-02
22 W(LIQUID,A)=0.187             0.1867      2.00E-02 -2.9105E-04 -1.4553E-02
22 W(FCC,A)=5.9E-2               5.9414E-02  2.00E-02  4.1416E-04  2.0708E-02
23 W(LIQUID,A)=0.245             0.2448      2.00E-02 -2.4851E-04 -1.2425E-02
23 W(BCC#1,A)=8.5E-2             8.5315E-02  2.00E-02  3.1454E-04  1.5727E-02
100 ACR(B)=0.94                  0.9397      2.85E-02 -2.7275E-04 -9.5825E-03
101 ACR(B)=0.84                  0.8395      2.82E-02 -4.7358E-04 -1.6802E-02
102 ACR(B)=0.74                  0.7408      2.81E-02  7.7139E-04  2.7496E-02
103 ACR(B)=0.64                  0.6424      2.81E-02  2.4449E-03  8.7112E-02
104 ACR(B)=0.54                  0.5435      2.82E-02  3.5129E-03  0.1245
105 ACR(B)=0.44                  0.4429      2.85E-02  2.9062E-03  0.1018
106 ACR(B)=0.34                  0.3395      2.90E-02 -4.9853E-04 -1.7174E-02
107 ACR(B)=0.23                  0.2321      2.97E-02  2.1003E-03  7.0704E-02
108 ACR(B)=0.12                  0.1194      3.06E-02 -5.9355E-04 -1.9397E-02
110 HMR(LIQUID)=-1964            -1956.      5.00E+02   8.026      1.6052E-02
111 HMR(LIQUID)=-3500            -3477.      5.00E+02   22.71      4.5425E-02
112 HMR(LIQUID)=-4588            -4564.      5.00E+02   24.06      4.8120E-02
```

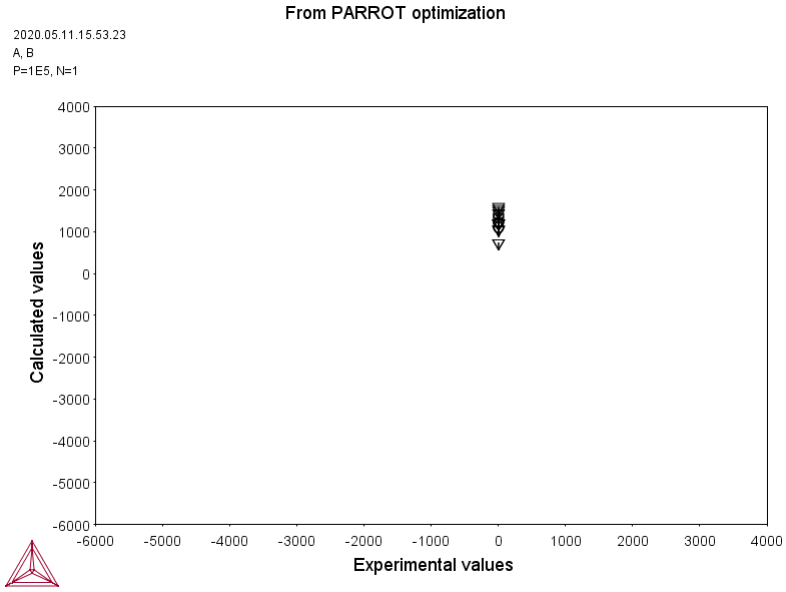
```
113 HMR(LIQUID)=-5239            -5216.      5.00E+02   23.07      4.6137E-02
114 HMR(LIQUID)=-5454            -5433.      5.00E+02   20.74      4.1476E-02
115 HMR(LIQUID)=-5233            -5216.      5.00E+02   17.07      3.4137E-02
116 HMR(LIQUID)=-4575            -4564.      5.00E+02   11.06      2.2120E-02
117 HMR(LIQUID)=-3481            -3477.      5.00E+02   3.712      7.4249E-03
118 HMR(LIQUID)=-1950            -1956.      5.00E+02  -5.974     -1.1948E-02


PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram one last time.
PARROT: mac tcex36cpd
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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   5 at:   3.771E-01  1.192E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.828E-01  1.192E+03
 ** LIQUID
    BCC#1
Calculated                      29 equilibria

Phase region boundary   7 at:   4.863E-01  1.192E+03
 ** LIQUID
    A2B
Calculated.                      28 equilibria

Phase region boundary   8 at:   6.500E-01  1.048E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.639E-01  1.048E+03
    A2B
 ** BCC#1
Calculated.                      11 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.272E-01  1.048E+03
    LIQUID
 ** BCC#1
Calculated.                       8 equilibria

Phase region boundary  11 at:   8.748E-01  1.203E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.799E-01  1.203E+03
    LIQUID
 ** FCC
Calculated                      33 equilibria

Phase region boundary  13 at:   9.353E-01  1.203E+03
    BCC#1
 ** FCC
Calculated                      22 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                      13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                       2 equilibria
Terminating at known equilibrium
```

```
 Terminating at axis limit.

 Phase region boundary  24 at:   7.140E-01  3.100E+02
  ** BCC#1
     BCC#2
 Calculated                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   3.647E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                      10 equilibria

 Phase region boundary  26 at:   3.647E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                       3 equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   3.647E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                      14 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.910E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                      10 equilibria

 Phase region boundary  29 at:   7.910E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                       3 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.910E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                       9 equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.448E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated                       4 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.448E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated                      26 equilibria

 Phase region boundary  33 at:   8.858E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                       2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.858E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                      29 equilibria

 Phase region boundary  35 at:   6.415E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated                      13 equilibria

 Phase region boundary  36 at:   6.415E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated                      13 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated                      20 equilibria

 Phase region boundary  38 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated                       4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated                      14 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated                       8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      20 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                      13 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     1 seconds
POLY: post
POST: s-l d
POST: plot
```

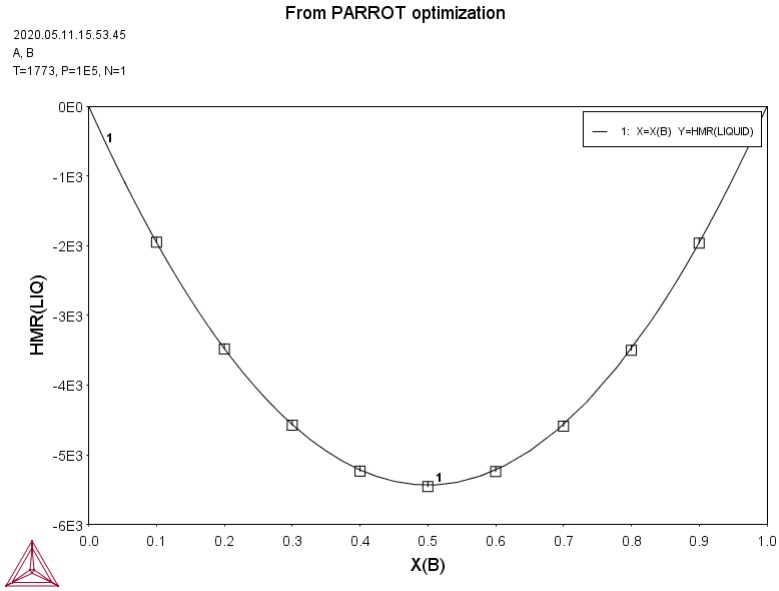



```
POST:
POST: set-inter
POST:Hit RETURN to continue
POST: @@ Add the experimental data
POST: a-e-d y exp36 0; 1
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
 *** ERROR  3004 IN LPOSTP:  NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

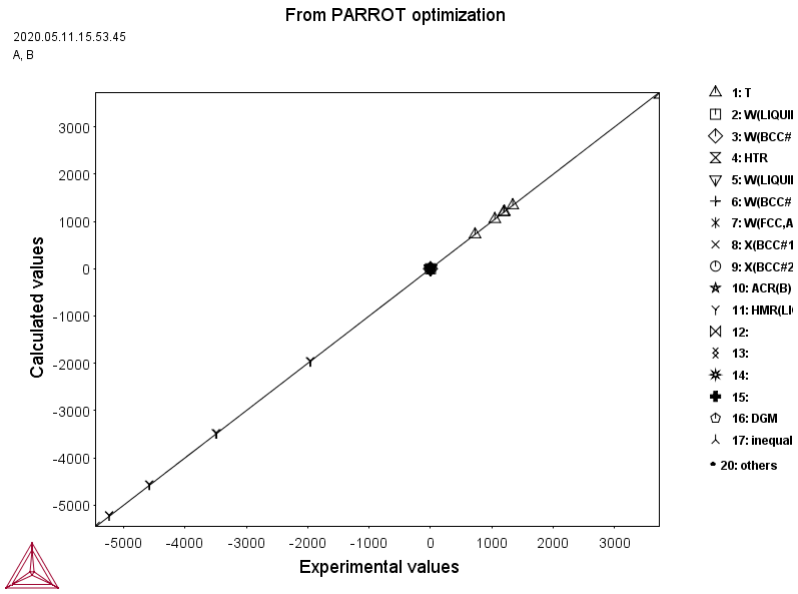



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
POLY: read,,,
POLY:
POLY:
POLY: s-a-v 2 none
POLY: s-c t=1773
POLY: c-e
 Using global minimization procedure
Calculated           628 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
POLY: sh hmr
 HMR=13116.464
POLY: l-st c
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)            P(Pa)
 A                        ENTERED   SER
 B                        ENTERED   SER
POLY: s-r-s a liq * 1e5
POLY: s-r-s b liq * 1e5
POLY: save tcex36h y

 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: step normal
 No initial equilibrium, using default
 Step will start from axis value   0.123400
...OK

 Phase Region from   0.123400     for:
```

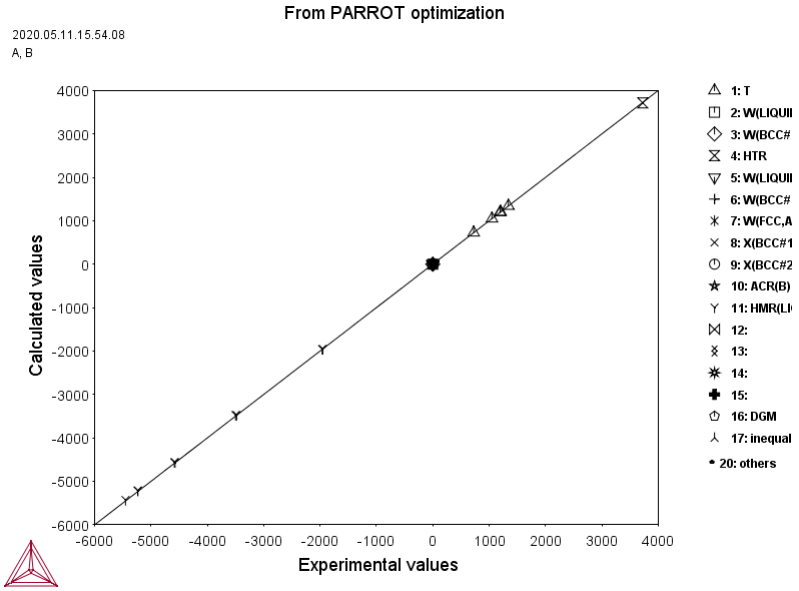
```
     LIQUID
 Global test at  3.23400E-01 .... OK
 Global test at  5.73400E-01 .... OK
 Global test at  8.23400E-01 .... OK
 Global test at  9.53400E-01 .... OK
 Global test at  1.00000E+00 .... OK
 Terminating at    1.00000
 Calculated    51 equilibria

 Phase Region from   0.123400     for:
     LIQUID
 Global test at  8.34000E-02 .... OK
 Global test at  3.34000E-02 .... OK
 Terminating at   0.250000E-11
 Calculated    28 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36h.POLY3
POLY: post
POST: s-d-a x x(b)
POST: s-d-a y hmr(liq)
POST: a-e-d y exp36 0; 2
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```




```
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
POLY: ba

 PARROT  VERSION 5.3

  Global minimization used as test only
PARROT: l-result gra pexp36 1,
```




```
POST: s-s-s y n -6000 4000
POST: s-s-s x n -6000 4000
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
 *** ERROR  3004 IN LPOSTP:  NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```



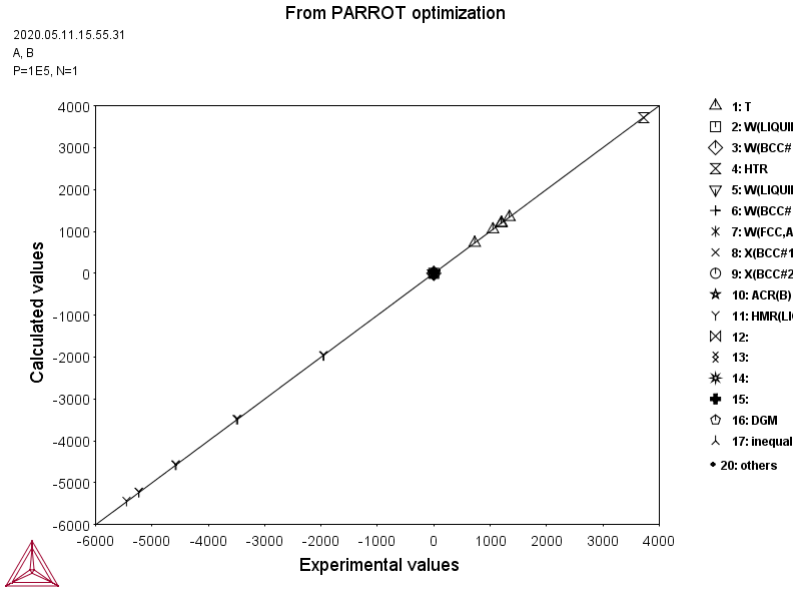

```
POST: b
PARROT: set-inter
PARROT:
```

tcex36a-tcex36cpd

```
PARROT:About
 NO SUCH COMMAND, USE HELP
PARROT:PARROT:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36cpd.TCM.test"
PARROT: set-echo
 NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
POLY:
POLY: @@ In PARROT, the global minimization is turned off automatically.
POLY: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY: @@ message will be given.
POLY:
POLY: advanced-option global yes,,
 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:
POLY: def-com,,,,
POLY: s-a-v 1 w(b) 0 1,,,,
 The condition W(B)=.1234  created
POLY: s-a-v 2 t 300 1700,,,,
 The condition T=942.2  created
POLY: s-c t=500
POLY: l-c
 W(B)=0.1234, T=500
 DEGREES OF FREEDOM 2
POLY: c-e
 Creating condition P=1E5
 Creating condition N=1
 Using global minimization procedure
Calculated           628 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: save tcex36 y

 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: 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   5 at:   3.771E-01  1.192E+03
 ** LIQUID
 ** A2B
    BCC#1

Phase region boundary   6 at:   2.828E-01  1.192E+03
 ** LIQUID
    BCC#1
Calculated                     29 equilibria

Phase region boundary   7 at:   4.863E-01  1.192E+03
 ** LIQUID
    A2B
Calculated.                     28 equilibria

Phase region boundary   8 at:   6.500E-01  1.048E+03
 ** LIQUID
    A2B
 ** BCC#1

Phase region boundary   9 at:   7.639E-01  1.048E+03
    A2B
 ** BCC#1
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  10 at:   8.272E-01  1.048E+03
    LIQUID
 ** BCC#1
Calculated.                      8 equilibria

Phase region boundary  11 at:   8.748E-01  1.203E+03
    LIQUID
 ** BCC#1
 ** FCC

Phase region boundary  12 at:   8.799E-01  1.203E+03
    LIQUID
 ** FCC
Calculated                     33 equilibria

Phase region boundary  13 at:   9.353E-01  1.203E+03
    BCC#1
 ** FCC
Calculated                     22 equilibria

Phase region boundary  14 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  17 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  18 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   7.140E-01  3.100E+02
    BCC#1
 ** BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  22 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated..                      2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   7.140E-01  3.100E+02
 ** BCC#1
    BCC#2
Calculated.                     13 equilibria
Terminating at known equilibrium
```

```
 Phase region boundary  25 at:   3.647E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                     10 equilibria

 Phase region boundary  26 at:   3.647E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                     3 equilibria
 Terminating at known equilibrium

 Phase region boundary  27 at:   3.647E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                    14 equilibria
 Terminating at known equilibrium

 Phase region boundary  28 at:   7.910E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated                     10 equilibria

 Phase region boundary  29 at:   7.910E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                     3 equilibria
 Terminating at known equilibrium

 Phase region boundary  30 at:   7.910E-01  7.700E+02
  ** A2B
     BCC#1
 Calculated.                     9 equilibria
 Terminating at known equilibrium

 Phase region boundary  31 at:   2.448E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated.                     4 equilibria
 Terminating at known equilibrium

 Phase region boundary  32 at:   2.448E-01  1.230E+03
  ** LIQUID
     BCC#1
 Calculated                     26 equilibria

 Phase region boundary  33 at:   8.858E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated.                     2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   8.858E-01  1.230E+03
  ** LIQUID
     FCC
 Calculated                     29 equilibria

 Phase region boundary  35 at:   6.415E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated                     13 equilibria

 Phase region boundary  36 at:   6.415E-03  1.397E+03
     LIQUID
  ** BCC#1
 Calculated.                    13 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated                     20 equilibria

 Phase region boundary  38 at:   2.299E-01  1.244E+03
     LIQUID
  ** BCC#1
 Calculated.                     4 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated.                    14 equilibria
 Terminating at known equilibrium

 Phase region boundary  40 at:   6.122E-01  1.240E+03
     LIQUID
  ** A2B
 Calculated.                     8 equilibria
 Terminating at known equilibrium

 Phase region boundary  41 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated.                    20 equilibria
 Terminating at known equilibrium

 Phase region boundary  42 at:   9.927E-01  1.613E+03
     LIQUID
  ** FCC
 Calculated                     13 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex36a\tcex36.POLY3
 CPU time for mapping                     1 seconds
POLY: post
POST: s-l d
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
 *** ERROR  3004 IN LPOSTP:  NO AXIS DEFINED
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```




```
POST:
POST: set-inter
POST:
```

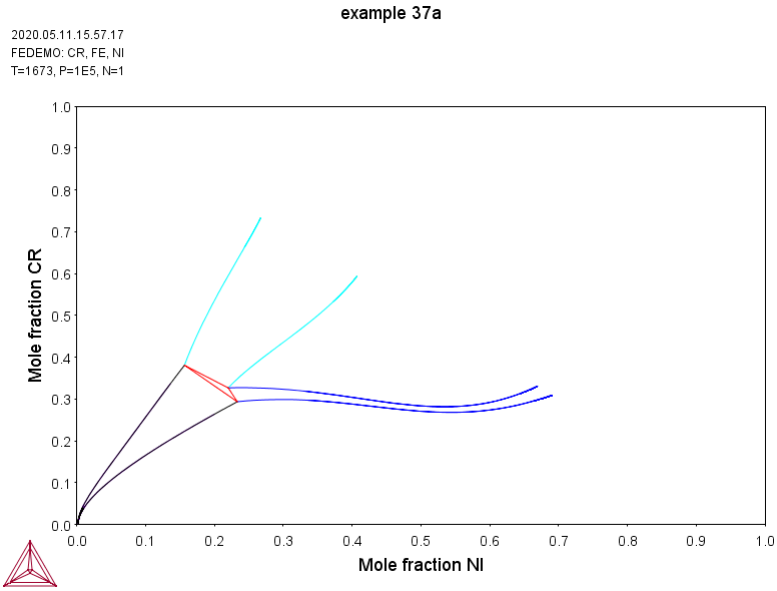
tcex37

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex37\tcex37.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculation of an isothermal section using command-lines
SYS:
SYS: @@ This example shows how use command lines to enter and
SYS: @@ calculate an isothermal section using the POLY3 module.
SYS: set-log tcex37,,
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                       /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw fedemo
   ... the command in full is SWITCH_DATABASE
 Current database: Iron Demo Database v3.0

 VA                       /-  DEFINED
TDB_FEDEMO: def-sys
   ... the command in full is DEFINE_SYSTEM
ELEMENTS: fe cr ni
 FE                       CR                       NI
   DEFINED
TDB_FEDEMO: l-s c
   ... the command in full is LIST_SYSTEM
 LIQUID:L    :CR FE NI:
 BCC_A2      :CR FE NI:VA:
 LAVES_PHASE_C14 :CR FE NI:CR FE NI:
 CBCC_A12    :CR FE NI:VA:
 CHI_A12     :CR FE NI:CR:CR FE NI:
 CUB_A13     :CR FE NI:VA:
 FCC_A1      :CR FE NI:VA:
 HCP_A3      :CR FE NI:VA:
 SIGMA       :CR FE NI:CR:CR FE NI:
TDB_FEDEMO:Hit RETURN to continue
TDB_FEDEMO: get
   ... the command in full is GET_DATA
15:57:10,656 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019'
  'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
  'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); CR -NI'
  'A.T. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.J. Lee, unpublished work at KTH (1999); update of steel database'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; C14_LAVES'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
      TCFE9 database (TCFE v9.0, Jan, 2017).'
  'Unassessed parameter; Linear combination of unary data'
  'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
       CR-FE-MO'
  'L.J. Zhang,Int.J. Mater. Res.,100(2) 160-175 (2009),Fe-Mn-Ni'
  'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'L.L. Zhu, H.Y. Qi, L. Jiang, Z.P. Jin, J.C. Zhao, Intermetallics. 64
      (2015) 86-95; Cr-Ru and Cr-Ni-Ru'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
  'R. Naraghi, Thermo-Calc Software AB, Sweden (2015); FROST project'
 -OK-
TDB_FEDEMO: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: cps
 *** STATUS FOR ALL COMPONENTS
```

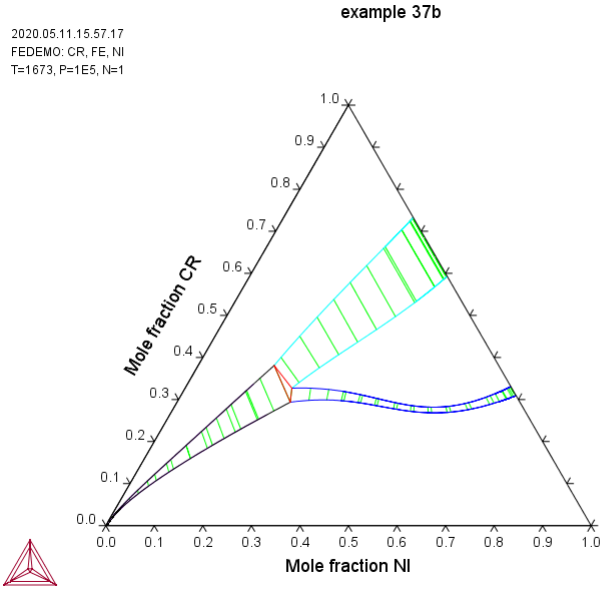
```
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 CR                       ENTERED   SER
 FE                       ENTERED   SER
 NI                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 SIGMA                    ENTERED      0.000000E+00    0.000000E+00
 LAVES_PHASE_C14          ENTERED      0.000000E+00    0.000000E+00
 HCP_A3                   ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                   ENTERED      0.000000E+00    0.000000E+00
 CUB_A13                  ENTERED      0.000000E+00    0.000000E+00
 CHI_A12                  ENTERED      0.000000E+00    0.000000E+00
 CBCC_A12                 ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                   ENTERED      0.000000E+00    0.000000E+00
 LIQUID                   ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 CR ENTERED    FE ENTERED    NI ENTERED    VA ENTERED
POLY: @@ Set conditions for a point inside the diagram

POLY: s-c x(cr)=0.2 x(ni)=0.4
   ... the command in full is SET_CONDITION
POLY: s-c t=1673 p=1e5 n=1
   ... the command in full is SET_CONDITION
POLY: 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: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         15786 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: FEDEMO

 Conditions:
 X(CR)=0.2, X(NI)=0.4, T=1673, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1673.00 K (  1399.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.62140E+01
 Total Gibbs energy -1.08423E+05,  Enthalpy  4.89973E+04,  Volume  7.34210E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 CR                       2.0000E-01  1.8499E-01 7.8623E-04 -9.9434E+04 SER
 FE                       4.0000E-01  3.9739E-01 4.0953E-04 -1.0851E+05 SER
 NI                       4.0000E-01  4.1762E-01 3.0004E-04 -1.1283E+05 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.6214E+01, Volume fraction 1.0000E+00  Mass fractions:
 NI  4.17618E-01  FE  3.97389E-01  CR  1.84993E-01
POLY: 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: 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: save tcex37 y
   ... the command in full is SAVE_WORKSPACES
POLY:
POLY: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

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

 Phase region boundary   1 at:   9.201E-03  4.019E-02
  ** BCC_A2
     FCC_A1
 Calculated                     14 equilibria

 Phase region boundary   2 at:   9.201E-03  4.019E-02
  ** BCC_A2
     FCC_A1
```

```
 Calculated.                     31 equilibria

 Phase region boundary   3 at:   1.950E-01  3.373E-01
  ** LIQUID
  ** BCC_A2
     FCC_A1

 Phase region boundary   4 at:   2.267E-01  3.103E-01
  ** LIQUID
     FCC_A1
 Calculated                     53 equilibria

 Phase region boundary   5 at:   1.883E-01  3.539E-01
  ** LIQUID
     BCC_A2
 Calculated                     49 equilibria

 Phase region boundary   6 at:   1.950E-01  3.373E-01
  ** BCC_A2
     FCC_A1
 Calculated                     51 equilibria

 Phase region boundary   7 at:   3.334E-01  3.082E-01
  ** LIQUID
     FCC_A1
 Calculated.                     10 equilibria
 Terminating at known equilibrium

 Phase region boundary   8 at:   3.334E-01  3.082E-01
  ** LIQUID
     FCC_A1
 Calculated                     39 equilibria

 Phase region boundary   9 at:   6.543E-01  3.046E-01
  ** LIQUID
     FCC_A1
 Calculated.                     35 equilibria
 Terminating at known equilibrium

 Phase region boundary  10 at:   6.543E-01  3.046E-01
  ** LIQUID
     FCC_A1
 Calculated                     23 equilibria

 Phase region boundary  11 at:   1.678E-01  3.000E-01
     BCC_A2
  ** FCC_A1
 Calculated                     34 equilibria

 Phase region boundary  12 at:   1.678E-01  3.000E-01
     BCC_A2
  ** FCC_A1
 Calculated.                      4 equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   3.086E-01  5.984E-01
  ** LIQUID
     BCC_A2
 Calculated.                     21 equilibria
 Terminating at known equilibrium

 Phase region boundary  14 at:   3.086E-01  5.984E-01
  ** LIQUID
     BCC_A2
 Calculated                     25 equilibria

 Phase region boundary  15 at:   1.097E-02  4.525E-02
     BCC_A2
  ** FCC_A1
 Calculated                     15 equilibria

 Phase region boundary  16 at:   1.097E-02  4.525E-02
     BCC_A2
  ** FCC_A1
 Calculated.                     31 equilibria
 Terminating at known equilibrium

 Phase region boundary  17 at:   3.342E-01  6.558E-01
     LIQUID
  ** BCC_A2
 Calculated.                     26 equilibria
 Terminating at known equilibrium

 Phase region boundary  18 at:   3.342E-01  6.558E-01
     LIQUID
  ** BCC_A2
 Calculated                     13 equilibria

 Phase region boundary  19 at:   6.736E-01  3.160E-01
     LIQUID
  ** FCC_A1
 Calculated.                     37 equilibria
 Terminating at known equilibrium

 Phase region boundary  20 at:   6.736E-01  3.160E-01
     LIQUID
  ** FCC_A1
 Calculated                     18 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex37\tcex37.POLY3
 CPU time for mapping                    7 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: @@ Use default axis on the diagram
POST:
POST: set-title example 37a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

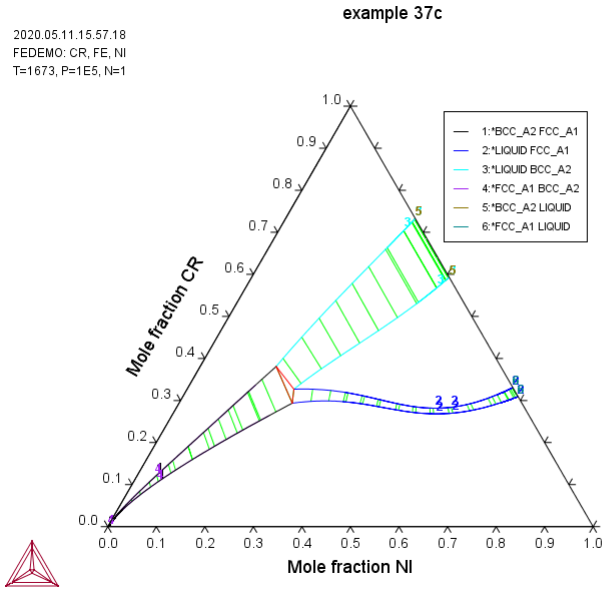
```
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ By default a diagram is always square. set it triangular,
POST: @@ add tie-lines and set scaling on the axis
POST: s-d-t
   ... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM  (Y OR N) /N/: y
POST: s-t-s
   ... the command in full is SET_TIELINE_STATUS
PLOTTING EVERY TIE-LINE NO /0/: 3
POST: s-sc
   ... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING  (Y OR N) /N/: n
MIN VALUE : 0
MAX VALUE : 1
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 37b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ To identify the phases also set labels
POST: @@ To add text in phase regions use a dataplot file
POST: set-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 37c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



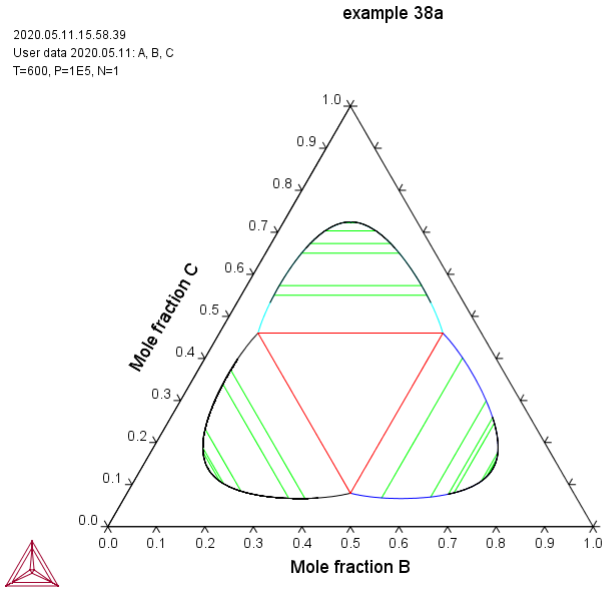

```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex38

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex38\tcex38.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating the Morral *rose*
SYS:
SYS: @@ This example uses the Gibbs energy system
SYS: @@ (GES) module to calculate the Morral rose,
SYS: @@ which are miscibility gaps.
SYS:
SYS: set-log ex38,,,,
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
15:58:33,772 INFO  *** Invoking Gibbs Energy System v6 ***
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
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
GES: a-e-d a fcc_a1 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d b fcc_a1 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d c fcc_a1 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES:
GES:
GES: e-ph fcc_a1,,1 A B C;,,,,,
   ... the command in full is ENTER_PHASE
GES:
GES:
GES: e-par l(fcc_a1,a,b,c),,50000;,,,,
   ... the command in full is ENTER_PARAMETER
 L(FCC_A1,A,B,C;0)
GES: l-d
   ... the command in full is LIST_DATA
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

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


 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
  1 A    FCC_A1                    1.0000E+01  0.0000E+00  0.0000E+00
  2 B    FCC_A1                    1.0000E+01  1.2220E+03  5.9000E+00
  3 C    FCC_A1                    1.0000E+01  1.0540E+03  5.7400E+00


 SPECIES                                     STOICHIOMETRY
   1 A                                       A
   2 B                                       B
   3 C                                       C



 FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B,C

      G(FCC_A1,A;0)-G(FCC_A1,A;0) = 0.0
      G(FCC_A1,B;0)-G(FCC_A1,B;0) = 0.0
      G(FCC_A1,C;0)-G(FCC_A1,C;0) = 0.0
      L(FCC_A1,A,B,C;0) = +50000

 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:

POLY: s-c t=600 p=1e5 n=1 x(b)=.3 x(c)=.1
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
15:58:35,609 INFO  Preparing system for use: UNKNOWN_1589205513822
15:58:36,139 INFO  Preparing phase for use: FCC_A1
Calculated          1965 grid points in             2 s
Found the set of lowest grid points in              0 s
 Creating a new composition set FCC_A1#2
 Calculated POLY solution       0 s, total time     2  s
```

```
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=600, P=1E5, N=1, X(B)=0.3, X(C)=0.1
 DEGREES OF FREEDOM 0

 Temperature    600.00 K (   326.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -3.58989E+03,  Enthalpy  6.74567E+02,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 A                       6.0000E-01  6.0000E-01 5.7356E-01 -2.7732E+03 SER
 B                       3.0000E-01  3.0000E-01 3.8092E-01 -4.8149E+03 SER
 C                       1.0000E-01  1.0000E-01 3.8092E-01 -4.8149E+03 SER

 FCC_A1#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_A1#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.2219E-01, Mass 1.2219E+00, Volume fraction 0.0000E+00  Mass fractions:
 A  6.00000E-01  C  3.32342E-01  B  6.76579E-02
POLY:Hit RETURN to continue
POLY: s-a-v 1 x(b) 0 1 0.01
   ... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 x(c) 0 1 0.01
   ... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: save tcex38 y
   ... the command in full is SAVE_WORKSPACES
POLY:
POLY: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Trying global minimization! 3
 Generating start point   1
 Generating start point   2
 Trying global minimization! 3
 Generating start point   3
 Generating start point   4
 Trying global minimization! 3
 Generating start point   5
 Generating start point   6
 Trying global minimization! 3
 Generating start point   7
 Generating start point   8
 Trying global minimization! 3
 Generating start point   9
 Generating start point  10
 Working hard
 Trying global minimization! 3
 Generating start point  11
 Generating start point  12

 Phase region boundary   1 at:   2.333E-01  2.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                     32 equilibria

 Phase region boundary   2 at:   2.333E-01  2.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Creating a new composition set FCC_A1#3
 Calculated                     10 equilibria

 Phase region boundary   3 at:   2.333E-01  2.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated.                      5 equilibria

 Phase region boundary   4 at:   2.699E-01  2.699E-01
     FCC_A1#1
  ** FCC_A1#2
  ** FCC_A1#3

 Phase region boundary   5 at:   4.603E-01  2.699E-01
     FCC_A1#1
  ** FCC_A1#3
 Calculated                     48 equilibria

 Phase region boundary   6 at:   2.699E-01  4.603E-01
     FCC_A1#2
  ** FCC_A1#3
 Calculated                     44 equilibria

 Phase region boundary   7 at:   2.699E-01  2.699E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                     36 equilibria

 Phase region boundary   8 at:   6.633E-01  1.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                     26 equilibria

 Phase region boundary   9 at:   6.633E-01  1.683E-01
     FCC_A1#1
  ** FCC_A1#2
```

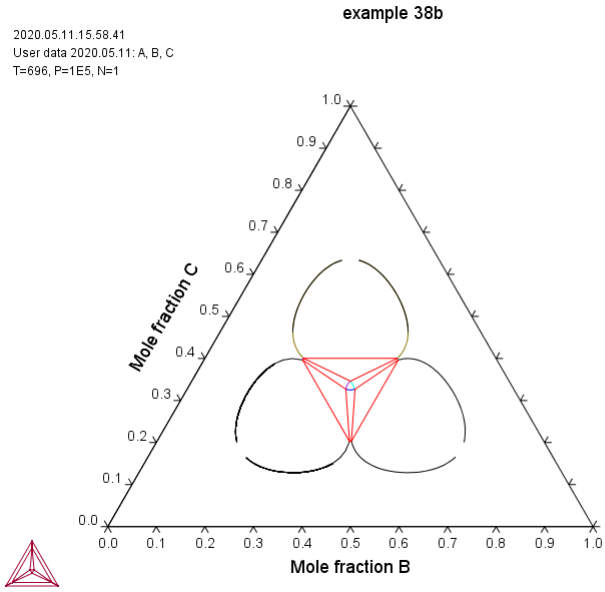
```
 Calculated                      33 equilibria

 Phase region boundary  10 at:   6.633E-01  1.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated.                      22 equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   2.333E-01  2.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      39 equilibria

 Phase region boundary  12 at:   2.333E-01  2.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      10 equilibria

 Phase region boundary  13 at:   2.333E-01  2.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated.                       5 equilibria
 Terminating at known equilibrium

 Phase region boundary  14 at:   1.683E-01  6.633E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      32 equilibria

 Phase region boundary  15 at:   1.683E-01  6.633E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated.                      22 equilibria
 Terminating at known equilibrium

 Phase region boundary  16 at:   1.683E-01  6.633E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      30 equilibria

 Phase region boundary  17 at:   2.333E-01  5.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      19 equilibria

 Phase region boundary  18 at:   2.333E-01  5.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated.                       9 equilibria
 Terminating at known equilibrium

 Phase region boundary  19 at:   2.333E-01  5.333E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      43 equilibria

 Phase region boundary  20 at:   6.633E-01  1.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      27 equilibria

 Phase region boundary  21 at:   6.633E-01  1.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      33 equilibria

 Phase region boundary  22 at:   6.633E-01  1.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated.                      22 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex38\tcex38.POLY3
 CPU time for mapping                      3 seconds
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST: s-d-a x m-f b
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y m-f c
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-t-s 10
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 38a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 Creating a new composition set FCC_A1#3
 The composition set FCC_A1#4 created from the store file
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: back
POLY: read,,
   ... the command in full is READ_WORKSPACES
POLY:
POLY: @@ We will calculate at a higher temperature
POLY: @@ with a stable phase in the middle.
POLY: s-c t=696
   ... the command in full is SET_CONDITION
POLY: s-c x(b)=.44 x(c)=.28
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1965 grid points in             0 s
Found the set of lowest grid points in              0 s
 Creating a new composition set FCC_A1#3
 Calculated POLY solution       0 s, total time     0  s
POLY:
POLY: save tcex38b y
   ... the command in full is SAVE_WORKSPACES
POLY:
POLY:
POLY: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9

 Organizing start points

Using ADDED start equilibria

 Working hard
 Trying global minimization! 3
 Generating start point   1
 Generating start point   2
 Trying global minimization! 3
 Generating start point   3
 Generating start point   4
 Trying global minimization! 3
 Generating start point   5
 Generating start point   6

 Phase region boundary   1 at:   2.683E-01  2.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                     35 equilibria

 Phase region boundary   2 at:   2.683E-01  2.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      6 equilibria

 Phase region boundary   3 at:   2.683E-01  2.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      6 equilibria

 Phase region boundary   4 at:   2.683E-01  2.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      6 equilibria

 Phase region boundary   5 at:   2.683E-01  2.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      6 equilibria

 Phase region boundary   6 at:   2.683E-01  2.683E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      6 equilibria

 Phase region boundary   7 at:   2.683E-01  2.683E-01
```

```
    FCC_A1#1
 ** FCC_A1#2
Calculated.                      6 equilibria

Phase region boundary   8 at:   2.998E-01  2.998E-01
    FCC_A1#1
 ** FCC_A1#2
 ** FCC_A1#3

Phase region boundary   9 at:   3.618E-01  2.650E-01
    FCC_A1#1
 ** FCC_A1#3
Calculated                       7 equilibria

Phase region boundary  10 at:   3.618E-01  2.650E-01
    FCC_A1#1
 ** FCC_A1#3
Calculated.                      5 equilibria

Phase region boundary  11 at:   3.732E-01  2.650E-01
    FCC_A1#1
 ** FCC_A1#2
 ** FCC_A1#3

Phase region boundary  12 at:   4.004E-01  2.998E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                      45 equilibria

Phase region boundary  13 at:   3.732E-01  3.618E-01
 ** FCC_A1#2
    FCC_A1#3
Calculated                       4 equilibria

Phase region boundary  14 at:   3.732E-01  3.618E-01
 ** FCC_A1#2
    FCC_A1#3
Calculated.                      3 equilibria

Phase region boundary  15 at:   3.618E-01  3.732E-01
 ** FCC_A1#1
 ** FCC_A1#2
    FCC_A1#3

Phase region boundary  16 at:   2.650E-01  3.732E-01
 ** FCC_A1#1
    FCC_A1#3
Calculated                       9 equilibria

Phase region boundary  17 at:   2.650E-01  3.732E-01
 ** FCC_A1#1
    FCC_A1#3
Calculated.                      7 equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   2.998E-01  4.004E-01
 ** FCC_A1#1
    FCC_A1#2
Calculated                      45 equilibria

Phase region boundary  19 at:   2.998E-01  2.998E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                      29 equilibria

Phase region boundary  20 at:   2.683E-01  2.683E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                      35 equilibria

Phase region boundary  21 at:   2.683E-01  2.683E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                       6 equilibria

Phase region boundary  22 at:   2.683E-01  2.683E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                       6 equilibria

Phase region boundary  23 at:   2.683E-01  2.683E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                       6 equilibria

Phase region boundary  24 at:   2.683E-01  2.683E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                       6 equilibria

Phase region boundary  25 at:   2.683E-01  2.683E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                       6 equilibria

Phase region boundary  26 at:   2.683E-01  2.683E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated.                      6 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   2.683E-01  4.633E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                       9 equilibria

Phase region boundary  28 at:   2.683E-01  4.633E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                       9 equilibria

Phase region boundary  29 at:   2.683E-01  4.633E-01
    FCC_A1#1
 ** FCC_A1#2
Calculated                       9 equilibria
```

```
 Phase region boundary  30 at:   2.683E-01  4.633E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      9 equilibria

 Phase region boundary  31 at:   2.683E-01  4.633E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                      9 equilibria

 Phase region boundary  32 at:   2.683E-01  4.633E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated.                      9 equilibria
 Terminating at known equilibrium

 Phase region boundary  33 at:   2.683E-01  4.633E-01
     FCC_A1#1
  ** FCC_A1#2
 Calculated                     44 equilibria
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex38\tcex38b.POLY3
 CPU time for mapping                     2 seconds
POLY:
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST:
POST: set-title example 38b
POST: s-d-ty y,,,,
   ... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
   ... the command in full is SET_SCALING_STATUS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

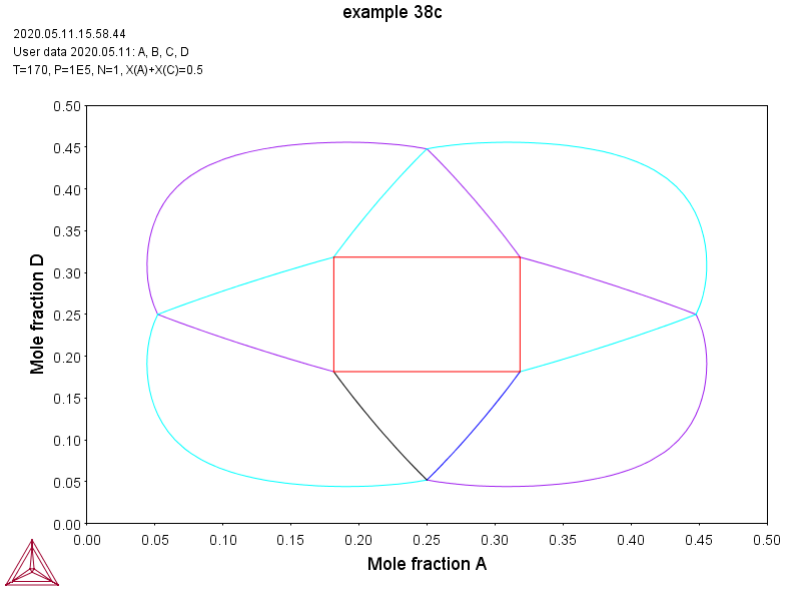



```
POST:
POST:Hit RETURN to continue
POST:
POST: back
POLY: @@ ==========================================
POLY: @@ Now a quaternary.
POLY: @@
POLY: @@ Square rose by John Morral
POLY: @@
POLY: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
GES: rei,,,,,
   ... the command in full is REINITIATE
GES: e-e a b c d
   ... the command in full is ENTER_ELEMENT
GES: a-e-d a liquid 10,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d b liquid 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d c liquid 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d d liquid 10,,,,,
   ... the command in full is AMEND_ELEMENT_DATA
GES: e-ph liquid
   ... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B C D
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES: e-par g(liquid,a,b,c,d)
```

```
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A,B,C,D;0)
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: 100000
&
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: N
GES:
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: rei,,,,
   ... the command in full is REINITIATE_MODULE
POLY: 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: 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:
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
15:58:41,405 INFO  Preparing system for use: UNKNOWN_1589205521240
15:58:41,529 INFO  Preparing phase for use: LIQUID
 Testing POLY result by global minimization procedure
Calculated          1787 grid points in             0 s
 Creating a new composition set LIQUID#2
    32 ITS,  CPU TIME USED   1 SECONDS
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VXCS
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=170, P=1E5, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
 DEGREES OF FREEDOM 0

 Temperature    170.00 K (  -103.15 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -1.58399E+03,  Enthalpy  2.18612E+02,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       3.0000E-01  3.0000E-01 3.1587E-01 -1.6289E+03 SER
 B                       2.5000E-01  2.5000E-01 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: 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: 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:
POLY: add +1
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY:
POLY: save tcex38c y
   ... the command in full is SAVE_WORKSPACES
POLY: 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   4 at:   2.500E-01  5.217E-02
     LIQUID#1
  ** LIQUID#2
     LIQUID#3
 Creating a new composition set LIQUID#4
 Calculated                     31 equilibria

 Phase region boundary   5 at:   2.500E-01  5.217E-02
     LIQUID#1
  ** LIQUID#2
     LIQUID#3
 Calculated.                     15 equilibria

 Phase region boundary   6 at:   1.816E-01  1.816E-01
```

```
    LIQUID#1
 ** LIQUID#2
    LIQUID#3
 ** LIQUID#4

Phase region boundary   7 at:   3.184E-01  1.816E-01
    LIQUID#1
    LIQUID#2
 ** LIQUID#3
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary   8 at:   3.184E-01  1.816E-01
    LIQUID#1
    LIQUID#2
 ** LIQUID#4
Calculated.                     14 equilibria

Phase region boundary   9 at:   4.478E-01  2.500E-01
 ** LIQUID#1
    LIQUID#2
 ** LIQUID#4

Phase region boundary  10 at:   4.478E-01  2.500E-01
    LIQUID#2
 ** LIQUID#4
Calculated.                     40 equilibria

Phase region boundary  11 at:   2.500E-01  4.478E-01
 ** LIQUID#1
    LIQUID#2
 ** LIQUID#4

Phase region boundary  12 at:   2.500E-01  4.478E-01
    LIQUID#1
    LIQUID#2
 ** LIQUID#4
Calculated                     20 equilibria

Phase region boundary  13 at:   2.500E-01  4.478E-01
    LIQUID#1
    LIQUID#2
 ** LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary  14 at:   2.500E-01  4.478E-01
 ** LIQUID#1
    LIQUID#2
Calculated.                     41 equilibria

Phase region boundary  15 at:   5.217E-02  2.500E-01
 ** LIQUID#1
    LIQUID#2
 ** LIQUID#4

Phase region boundary  16 at:   5.217E-02  2.500E-01
 ** LIQUID#1
    LIQUID#2
    LIQUID#4
Calculated                     20 equilibria

Phase region boundary  17 at:   5.217E-02  2.500E-01
 ** LIQUID#1
    LIQUID#2
    LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   5.217E-02  2.500E-01
    LIQUID#2
 ** LIQUID#4
Calculated.                     41 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   5.217E-02  2.500E-01
    LIQUID#1
    LIQUID#2
 ** LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary  20 at:   2.500E-01  4.478E-01
 ** LIQUID#1
    LIQUID#2
    LIQUID#4
Calculated                     20 equilibria

Phase region boundary  21 at:   2.500E-01  4.478E-01
 ** LIQUID#1
    LIQUID#2
    LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   4.478E-01  2.500E-01
 ** LIQUID#1
    LIQUID#2
Calculated.                     41 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   4.478E-01  2.500E-01
 ** LIQUID#1
    LIQUID#2
    LIQUID#4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary  24 at:   4.478E-01  2.500E-01
    LIQUID#1
 ** LIQUID#2
Calculated                      6 equilibria

Phase region boundary  25 at:   4.478E-01  2.500E-01
    LIQUID#1
 ** LIQUID#2
```

```
 Calculated                      2 equilibria

 Phase region boundary  26 at:   4.478E-01  2.500E-01
     LIQUID#1
  ** LIQUID#2
 Calculated                      2 equilibria

 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                      2 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: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex38\tcex38c.POLY3
 CPU time for mapping                      2 seconds
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:
POST:
POST: set-title example 38c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 Creating a new composition set LIQUID#3
 The composition set LIQUID#5 created from the store file
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

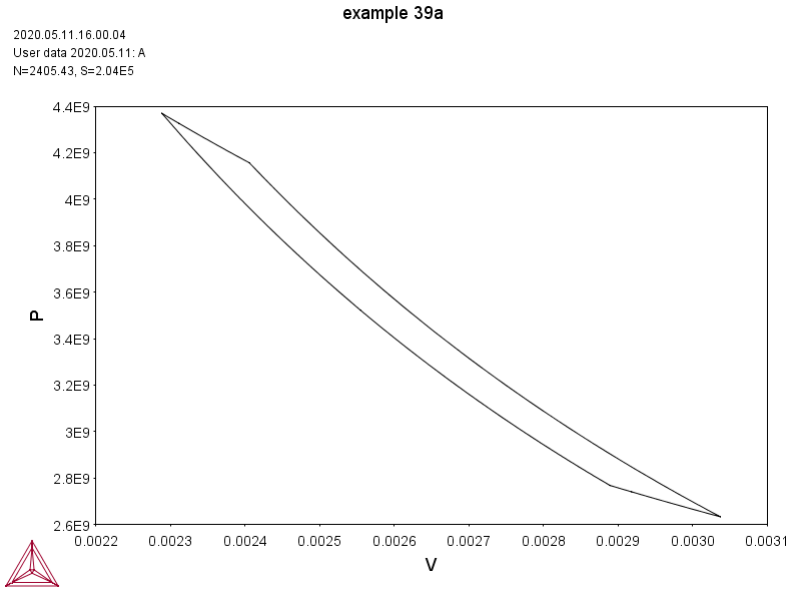
tcex39

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculating reversible Carnot cycles of a heat engine
SYS:
SYS: @@ This example shows how to calculate the reversible
SYS: @@ Carnot cycle of a heat engine using one mole of an ideal
SYS: @@ gas with two fictitious species A and A2. The GES, POLY3
SYS: @@ and POST modules are used.
SYS:
SYS: @@ One application of the Second Law is to the efficiencies
SYS: @@ of heat engines, pumps and refrigerators. Whenever there
SYS: @@ is a difference of temperature, work can be produced -
SYS: @@ the principle of heat engines. The Gibbs energy also
SYS: @@ enables the prediction of the maximum work that a process
SYS: @@ may achieve. The goal of this example is to help relate
SYS: @@ the results to different thermodynamic quantities.
SYS:
SYS: set-log ex39,,,
SYS:
SYS: go g
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
15:59:59,910 INFO  *** Invoking Gibbs Energy System v6 ***
GES: rei,,,,,
   ... the command in full is REINITIATE
GES: e-e a
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 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 species could be described
GES: @@ by the general formula: Gm= a +bT + cTlnT + dT2 +...+ RTln(P)
GES:
GES: @@ To calculate the Carnot cycle you have 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
GES: @@ be chosen arbitrarily, for example c should be negative as
GES: @@ the heat capacity at constant pressure, Cp = - T d2G/dT2
GES: @@ and thus Cp=-c-2dT, must always be >0
GES:
GES: e-par g(gas,a) 298.15 6960-51*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,,
   ... the command in full is ENTER_PARAMETER
 G(GAS,A;0)-G(GAS,A;0)
GES: e-par g(gas,a2) 298.15 130670-38*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,,
   ... the command in full is ENTER_PARAMETER
 G(GAS,A2;0)- 2 G(GAS,A;0)
GES: l-d,,,,
   ... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

 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
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


GES:Hit RETURN to continue
GES: @@ The Carnot cycle diagram gives the pressure and volume for
GES: @@ the working media of a heat engine that operates between
GES: @@ two temperatures T1 and T2, T1>T2.
GES:
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
```

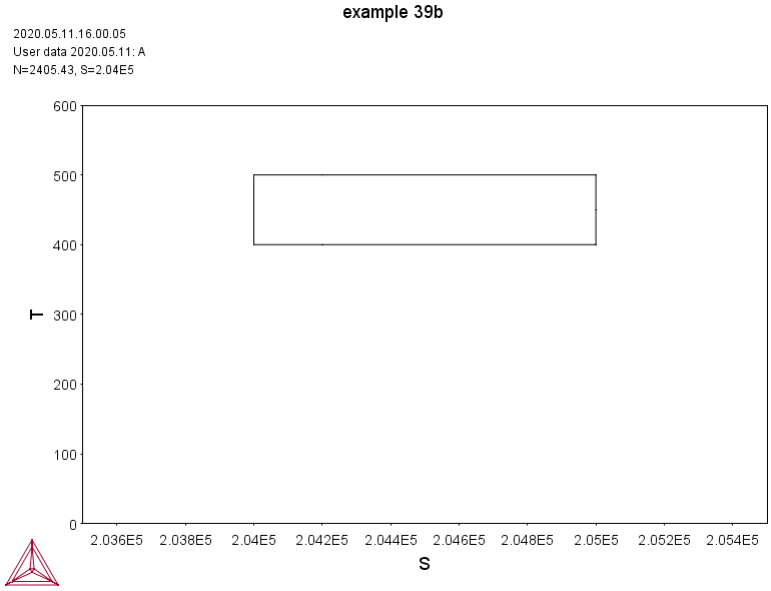
```
POLY: @@ The Carnot cycle is calculated for T1=500 K (the

POLY: @@ temperature of the hot reservoir) and T2=400 K
POLY: @@ (the temperature of the cold reservoir)
POLY: ent var t1=500;
   ... the command in full is ENTER_SYMBOL
POLY: ent var t2=400;
   ... the command in full is ENTER_SYMBOL
POLY:
POLY: @@ A Carnot cycle consists of four reversible stages:
POLY:
POLY: @@ Stage 1. Isothermal expansion at T1; the entropy change
POLY: @@ of the system is Q1/T1, where Q1 is the heat taken from
POLY: @@ the hot reservoir.
POLY:
POLY: s-c t=t1 p=1e7 n=1
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
16:00:01,803 INFO  Preparing system for use: UNKNOWN_1589205599965
16:00:02,472 INFO  Preparing phase for use: GAS
 Using global minimization procedure
Calculated           209 grid points in             0 s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xn
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=T1, P=1E7, N=1
 DEGREES OF FREEDOM 0

 Temperature    500.00 K (   226.85 C),  Pressure  1.000000E+07
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -5.22193E+04,  Enthalpy  1.54600E+04,  Volume  4.15726E-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:Hit RETURN to continue
POLY: @@ Set volume to 1 m3
POLY: s-c v
   ... the command in full is SET_CONDITION
Value /4.157255E-04/: 1
POLY: s-c n
   ... the command in full is SET_CONDITION
Value /1/: none
POLY: 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: 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: s-c n
   ... the command in full is SET_CONDITION
Value /2405.433393/:
POLY: s-c p
   ... the command in full is SET_CONDITION
Value /10000000/: none
POLY: 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: 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: enter var ha=h;
   ... the command in full is ENTER_SYMBOL
POLY: enter var sa=s;
```

```
   ... the command in full is ENTER_SYMBOL
POLY: s-c s
   ... the command in full is SET_CONDITION
Value /325596.1064/: sa
POLY: s-c v=none
   ... the command in full is SET_CONDITION
POLY: 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: 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:Hit RETURN to continue
POLY: 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:Hit RETURN to continue
POLY: ent var ga=g;
   ... the command in full is ENTER_SYMBOL
POLY: ent var pa=p;
   ... the command in full is ENTER_SYMBOL
POLY: ent var va=v;
   ... the command in full is ENTER_SYMBOL
POLY: @@
POLY: @@
POLY: save tcex39a y
   ... the command in full is SAVE_WORKSPACES
POLY: s-c t=500
   ... the command in full is SET_CONDITION
POLY: s-c s=204200
   ... the command in full is SET_CONDITION
POLY: s-a-v 1 s 204000 205000,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           209 grid points in             0 s
    17 ITS,  CPU TIME USED   0 SECONDS
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    204200.
...OK

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04400E+05 .... OK
 Global test at  2.04650E+05 .... OK
 Global test at  2.04900E+05 .... OK
 Terminating at    205000.
 Calculated    35 equilibria

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04000E+05 .... OK
 Terminating at    204000.
 Calculated    11 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: @@ Stage 2. Adiabatic expansion. No heat leaves the system,
POLY: @@ so the change in its entropy is zero. In the course of
POLY: @@ this expansion the temperature falls from T1 to T2, the
POLY: @@ temperature of cold reservoir.
POLY:
POLY: s-c s=205000
   ... the command in full is SET_CONDITION
POLY: s-c t=450
   ... the command in full is SET_CONDITION
POLY: s-a-v 1 t 400 500,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           209 grid points in             0 s
    12 ITS,  CPU TIME USED   0 SECONDS
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
...OK

 Phase Region from    450.000     for:
     GAS
 Global test at  4.70000E+02 .... OK
 Global test at  4.95000E+02 .... OK
 Terminating at    500.000
```

```
 Calculated    23 equilibria

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Terminating at    400.000
 Calculated    23 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: @@ Stage 3. Isothermal compresion at T2. The heat Q2 is
POLY: @@ released to the cold reservoir, so the change in
POLY: @@ entropy of the system is -Q2/T2.
POLY:
POLY: s-c t=400
   ... the command in full is SET_CONDITION
POLY: s-c s=204200
   ... the command in full is SET_CONDITION
POLY: s-a-v 1 s 204000 205000,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           209 grid points in             0 s
     8 ITS,  CPU TIME USED   0 SECONDS
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    204200.
...OK

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04400E+05 .... OK
 Global test at  2.04650E+05 .... OK
 Global test at  2.04900E+05 .... OK
 Terminating at    205000.
 Calculated    35 equilibria

 Phase Region from    204200.     for:
     GAS
 Global test at  2.04000E+05 .... OK
 Terminating at    204000.
 Calculated    11 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: @@ Stage 4. Adiabatic compression. No heat enters the system,
POLY: @@ so the change in entropy is zero. The temperature rises
POLY: @@ from T2 to T1.
POLY:
POLY: s-c s=204000
   ... the command in full is SET_CONDITION
POLY: s-c t=450
   ... the command in full is SET_CONDITION
POLY: s-a-v 1 t 400 500,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           209 grid points in             0 s
    10 ITS,  CPU TIME USED   0 SECONDS
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
...OK

 Phase Region from    450.000     for:
     GAS
 Global test at  4.70000E+02 .... OK
 Global test at  4.95000E+02 .... OK
 Terminating at    500.000
 Calculated    23 equilibria

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Terminating at    400.000
 Calculated    23 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39a.POLY3
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST:Plotformat
POST:
POST: s-p-f ##1,,,,,,,,,,,
   ... the command in full is SET_PLOT_FORMAT
 CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



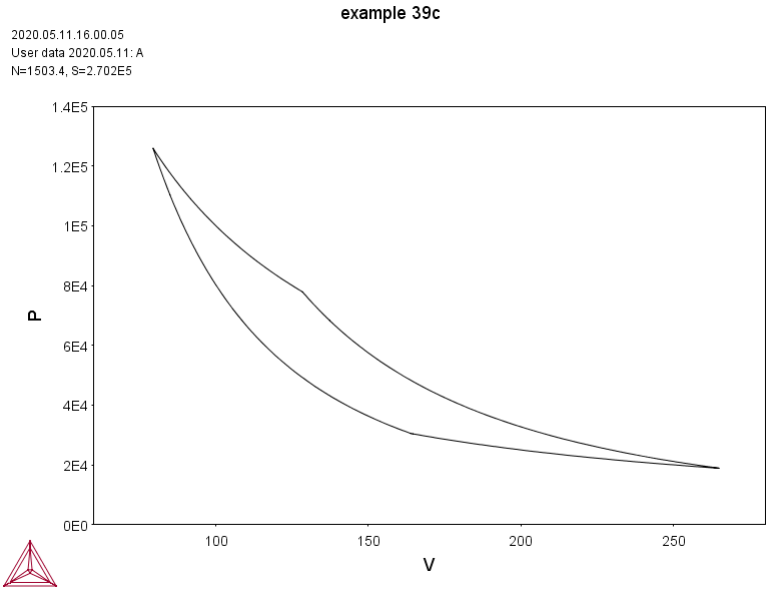

```
POST:
POST:Hit RETURN to continue
POST: @@ The efficiency E of an engine which uses a Carnot
POST: @@ cycle is:
POST: @@ E=work performed/heat absorbed = W/Q1
POST: @@ If you plot the entropy versus temperature, you can
POST: @@ calculate the work performed just by calculating the
POST: @@ area of the surface depicted by the two squares and
POST: @@ 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:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



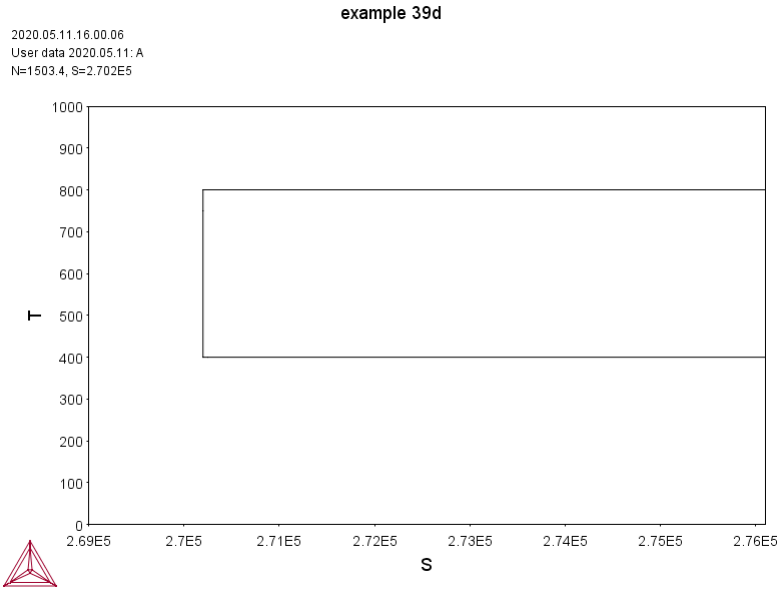

```
POST:
POST:Hit RETURN to continue
POST: @@ The influence of the value of the temperature T1 (the
POST: @@ temperature of the hot reservoir) on the efficency of the
POST: @@ Carnot cycle is important. Therefore we will make another
POST: @@ calculation for T1=800 K and compare with the one for
POST: @@ T1=500 K (example 39a and b). T2=400 K in both cases.
POST:
POST: ba
   ... the command in full is BACK
POLY: read,,,
   ... the command in full is READ_WORKSPACES
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=T1, N=2405.43, S=SA
 DEGREES OF FREEDOM 0
POLY: s-c s=none
   ... the command in full is SET_CONDITION
POLY: s-c t=800  p=1e7 n=1
   ... the command in full is SET_CONDITION
```

```
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           209 grid points in             0 s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=800, P=1E7, N=1
 DEGREES OF FREEDOM 0

 Temperature    800.00 K (   526.85 C),  Pressure  1.000000E+07
 Number of moles of components  1.00000E+00,  Mass in grams  1.00000E+01
 Total Gibbs energy -9.41189E+04,  Enthalpy  2.05600E+04,  Volume  6.65161E-04

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       1.0000E+00  1.0000E+00 7.1585E-07 -9.4119E+04 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00  Mole fractions:
 A  1.00000E+00
 Constitution:
 A   1.00000E+00  A2  1.27812E-15
POLY: @@ Set volume to 1 m3
POLY: s-c v
   ... the command in full is SET_CONDITION
Value /6.651608E-04/: 1
POLY: s-c n
   ... the command in full is SET_CONDITION
Value /1/: none
POLY: 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: s-c n
   ... the command in full is SET_CONDITION
Value /1503.395871/:
POLY: s-c p
   ... the command in full is SET_CONDITION
Value /10000000/: none
POLY: 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: enter var ha=h;
   ... the command in full is ENTER_SYMBOL
POLY: enter var sa=s;
   ... the command in full is ENTER_SYMBOL
POLY: s-c s
   ... the command in full is SET_CONDITION
Value /215509.7923/: sa
POLY: s-c v=none
   ... the command in full is SET_CONDITION
POLY: 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: 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:Hit RETURN to continue
POLY: save tcex39b y
   ... the command in full is SAVE_WORKSPACES
POLY: s-c s=272000
   ... the command in full is SET_CONDITION
POLY: s-a-v 1 s 270200 276200,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           209 grid points in             0 s
    53 ITS,  CPU TIME USED   0 SECONDS
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    272000.
...OK

 Phase Region from    272000.     for:
     GAS
 Global test at  2.73200E+05 .... OK
 Global test at  2.74700E+05 .... OK
 Global test at  2.76200E+05 .... OK
 Terminating at    276200.
 Calculated    31 equilibria

 Phase Region from    272000.     for:
     GAS
 Global test at  2.70800E+05 .... OK
 Terminating at    270200.
 Calculated    15 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c s=276200
   ... the command in full is SET_CONDITION
POLY: s-c t=750
   ... the command in full is SET_CONDITION
POLY: s-a-v 1 t 400 800,,,,
   ... the command in full is SET_AXIS_VARIABLE
```

```
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           209 grid points in             0 s
    13 ITS,  CPU TIME USED   0 SECONDS
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    750.000
...OK

 Phase Region from    750.000     for:
     GAS
 Terminating at    800.000
 Calculated     8 equilibria

 Phase Region from    750.000     for:
     GAS
 Global test at  6.70000E+02 .... OK
 Global test at  5.70000E+02 .... OK
 Global test at  4.70000E+02 .... OK
 Terminating at    400.000
 Calculated    38 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c t=400
   ... the command in full is SET_CONDITION
POLY: s-c s=270250
   ... the command in full is SET_CONDITION
POLY: s-a-v 1 s 270200 276200,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           209 grid points in             0 s
     9 ITS,  CPU TIME USED   0 SECONDS
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    270250.
...OK

 Phase Region from    270250.     for:
     GAS
 Global test at  2.71450E+05 .... OK
 Global test at  2.72950E+05 .... OK
 Global test at  2.74450E+05 .... OK
 Global test at  2.75950E+05 .... OK
 Terminating at    276200.
 Calculated    43 equilibria

 Phase Region from    270250.     for:
     GAS
 Terminating at    270200.
 Calculated     4 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY: s-c s=270200
   ... the command in full is SET_CONDITION
POLY: s-c t=750
   ... the command in full is SET_CONDITION
POLY: s-a-v 1 t 400 800,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Normal POLY minimization, not global
 Testing POLY result by global minimization procedure
Calculated           209 grid points in             0 s
    24 ITS,  CPU TIME USED   1 SECONDS
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    750.000
...OK

 Phase Region from    750.000     for:
     GAS
 Terminating at    800.000
 Calculated     8 equilibria

 Phase Region from    750.000     for:
     GAS
 Global test at  6.70000E+02 .... OK
 Global test at  5.70000E+02 .... OK
 Global test at  4.70000E+02 .... OK
 Terminating at    400.000
 Calculated    38 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39b.POLY3
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-p-f ##1,,,,,,,,,
   ... the command in full is SET_PLOT_FORMAT
 CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39c
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-d-a x s
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 269000 276100
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1000
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 39d
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

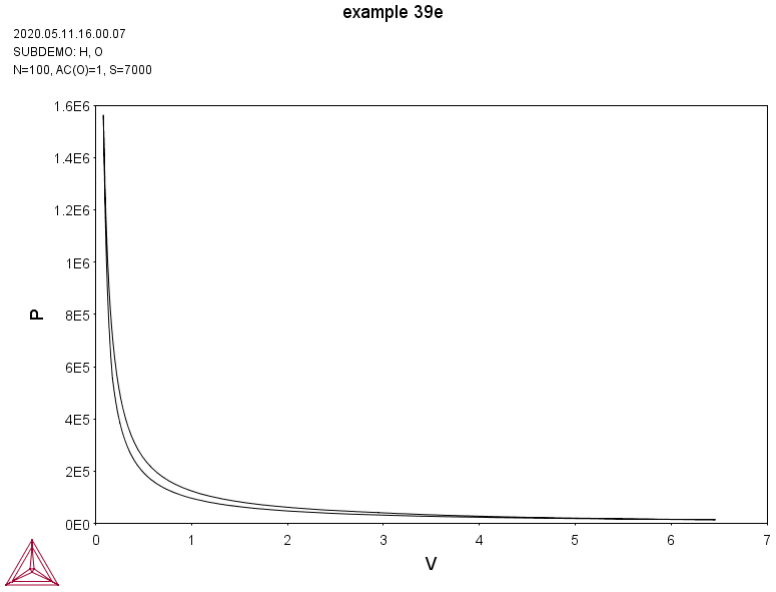



```
POST:
POST:Hit RETURN to continue
POST: @@ The efficiency for high value of T1 temperature is almost
POST: @@ double compared  with that one for low value of T1
POST: @@ temperature (compare plot examples 39b with example 39d).
POST:
POST: @@ Now we will calculate the Carnot cycle for some real systems.
POST: @@  The most 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: go da
   ... the command in full is GOTO_MODULE
TDB_TCFE10: rej sys
   ... the command in full is REJECT
 VA                        /-  DEFINED
 DICTRA_FCC_A1  REJECTED
 REINITIATING GES .....
TDB_TCFE10: sw subdemo
   ... the command in full is SWITCH_DATABASE
 Current database: Substance Demo Database v1.0

 VA                        /-  DEFINED
TDB_SUBDEMO: def-sp h2o1
   ... the command in full is DEFINE_SPECIES
 H2O1  DEFINED
TDB_SUBDEMO: l-sys
```

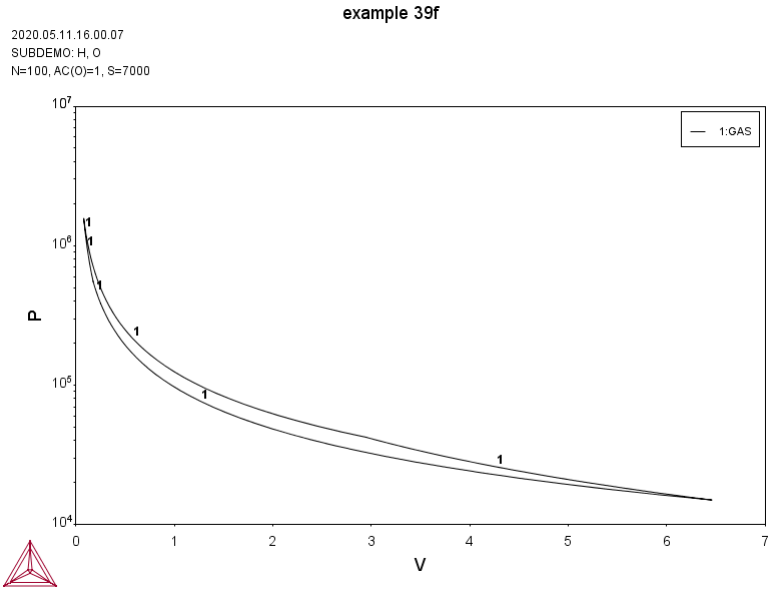
```
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
 GAS:G       :H2O1:
 H2O1_L      :H2O1:
TDB_SUBDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
  'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
 -OK-
TDB_SUBDEMO: @@ patch
TDB_SUBDEMO: go g-e-s
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
GES: li-st,,,,,
   ... the command in full is LIST_STATUS
 GAS CONSTANT IN USER ENERGY UNITS:      8.31451000E+00
 1 BAR IN USER PRESSURE UNITS:           1.00000000E+05
 CURRENT VALUE OF TEMPERATURE (KELVIN):          298.15
 CURRENT VALUE OF PRESSURE (PASCAL):     1.00000000E+05

 CURRENT NUMBER OF ELEMENT     4

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00 80000000
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00 80000000
  1 H    1/2_MOLE_H2(GAS)          1.0079E+00  4.2340E+03  6.5285E+01 08000000
  2 O    1/2_MOLE_O2(GAS)          1.5999E+01  4.3410E+03  1.0252E+02 08000000

 CURRENT NUMBER OF PHASE       2

 PHASE                          STATUS   SUBLATTICES
   1 GAS                        88200000     1
   2 H2O1_L                     82200000     1

 CURRENT NUMBER OF SPECIES     4

 SPECIES                                   STOICHIOMETRY
   1 H                           80800000   H
   2 H2O1                        00000000   H2O1
   3 O                           80800000   O
   4 VA                          81800000   VA

GES: @@ patch
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 H2O1_L                   ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY: c-st p h2o_l=sus
   ... the command in full is CHANGE_STATUS
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 H                        ENTERED   SER
 O                        ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 SUSPENDED PHASES:
 H2O1_L
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY: @@ The Carnot cycle will be calculated for T1=350 K and T2=450 K
POLY:
POLY: s-c t=380 p=1e5 n=100 ac(o)=1
   ... the command in full is SET_CONDITION
POLY: 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature    380.00 K (   106.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.04643E+07,  Enthalpy -7.96861E+06,  Volume  1.05317E+00

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 H                        6.6667E+01  6.6667E-01 2.6556E-22 -1.5697E+05 SER
 O                        3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER
```

```
 GAS                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY: s-c p=none
   ... the command in full is SET_CONDITION
POLY: s-c s
   ... the command in full is SET_CONDITION
Value /6567.729231/: 6100
POLY: s-c t=350
   ... the command in full is SET_CONDITION
POLY: 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: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 T=350, N=100, AC(O)=1, S=6100
 DEGREES OF FREEDOM 0

 Temperature    350.00 K (    76.85 C),  Pressure  3.863619E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.01376E+07,  Enthalpy -8.00259E+06,  Volume  2.51067E-01

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 H                        6.6667E+01  6.6667E-01 2.0244E-23 -1.5206E+05 SER
 O                        3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                        Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY: @@ step in S with t=350
POLY: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex39c y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
...OK

 Phase Region from    6100.00     for:
     GAS
 Global test at  6.30000E+03 .... OK
 Global test at  6.55000E+03 .... OK
 Global test at  6.80000E+03 .... OK
 Terminating at    7000.00
 Calculated    39 equilibria

 Phase Region from    6100.00     for:
     GAS
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY:
POLY: read,,,,
   ... the command in full is READ_WORKSPACES
POLY: s-c s=6000
   ... the command in full is SET_CONDITION
POLY: 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: @@ step in T with S=6000
POLY: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    350.000
...OK

 Phase Region from    350.000     for:
     GAS
 Global test at  3.70000E+02 .... OK
 Global test at  3.95000E+02 .... OK
 Global test at  4.20000E+02 .... OK
 Global test at  4.45000E+02 .... OK
 Terminating at    450.000
 Calculated    43 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: read,,,,
   ... the command in full is READ_WORKSPACES
POLY: s-c t=450
   ... the command in full is SET_CONDITION
POLY: 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: @@ Step in S with t=450
POLY: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
...OK
```

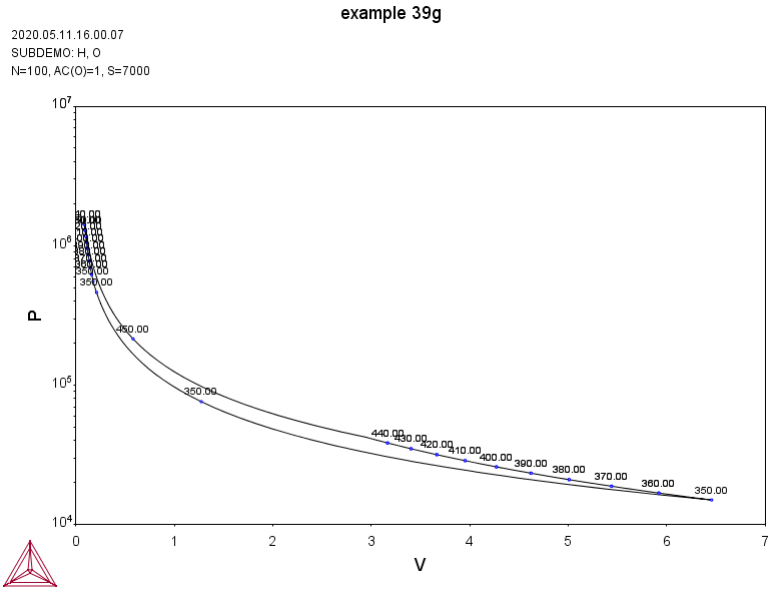
```
 Phase Region from    6100.00     for:
     GAS
 Global test at  6.30000E+03 .... OK
 Global test at  6.55000E+03 .... OK
 Global test at  6.80000E+03 .... OK
 Terminating at    7000.00
 Calculated    39 equilibria

 Phase Region from    6100.00     for:
     GAS
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: s-c s=7000
   ... the command in full is SET_CONDITION
POLY: 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: @@ Step in T with S=7000
POLY: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
...OK

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Global test at  3.80000E+02 .... OK
 Global test at  3.55000E+02 .... OK
 Terminating at    350.000
 Calculated    43 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39c.POLY3
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-p-f ##1,,,,,,,,
   ... the command in full is SET_PLOT_FORMAT
 CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39e
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39f
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ It is a bit difficult to distinguish from the calculated
POST: @@ diagram, example 39e, where the adiabatic expansion and
POST: @@ compresion start. Therefore it is good to plot temperature
POST: @@ on the same diagram.
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:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

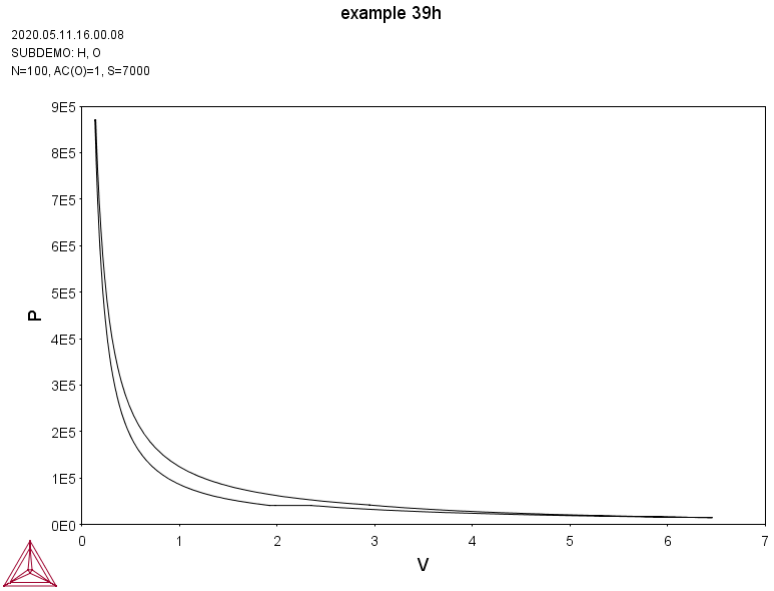



```
POST:
POST:Hit RETURN to continue
POST: @@ With Thermo-Calc you can also calculate the Carnot cycle
POST: @@ for real systems and include phase transformations.
POST:
POST: @@ Trying a Carnot cycle for water - it shows the case with
POST: @@ H2O_liquid to gas phase transformation. In the calculations
POST: @@  the volume of the liquid water is ignored.
POST:
POST: ba
   ... the command in full is BACK
POLY: go da
   ... the command in full is GOTO_MODULE
TDB_SUBDEMO: rej sys
   ... the command in full is REJECT
 VA                      /-  DEFINED
 REINITIATING GES .....
TDB_SUBDEMO: sw subdemo
   ... the command in full is SWITCH_DATABASE
TDB_SUBDEMO: def-sp h2o1
   ... the command in full is DEFINE_SPECIES
 H2O1  DEFINED
TDB_SUBDEMO: l-sys
   ... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
 GAS:G       :H2O1:
 H2O1_L      :H2O1:
```

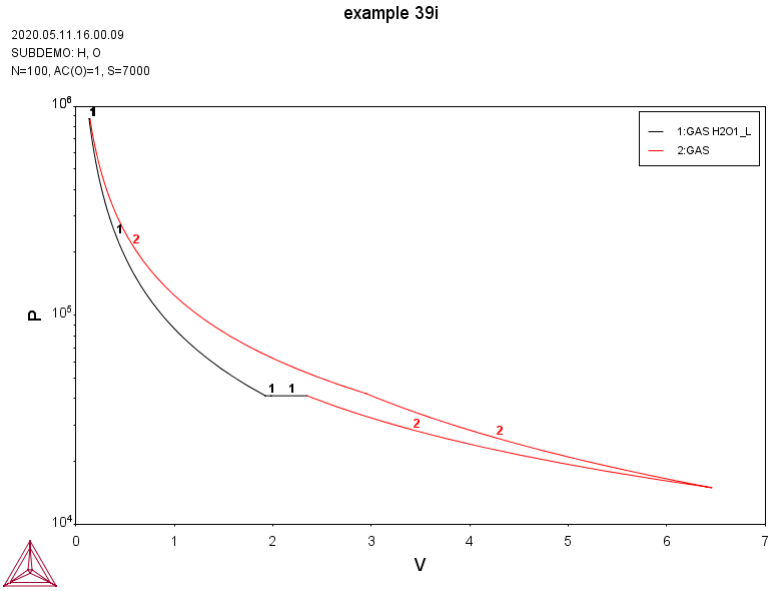
```
TDB_SUBDEMO: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
  'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure_Water WATER
      T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
 -OK-
TDB_SUBDEMO: @@ patch
TDB_SUBDEMO: go g-e-s
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
GES: li-st,,,,,
   ... the command in full is LIST_STATUS
 GAS CONSTANT IN USER ENERGY UNITS:      8.31451000E+00
 1 BAR IN USER PRESSURE UNITS:           1.00000000E+05
 CURRENT VALUE OF TEMPERATURE (KELVIN):          298.15
 CURRENT VALUE OF PRESSURE (PASCAL):     1.00000000E+05

 CURRENT NUMBER OF ELEMENT     4

 ELEMENT STABLE ELEMENT REFERENCE  MASS        H298-H0     S298
 -1 /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00 80000000
  0 VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00 80000000
  1 H    1/2_MOLE_H2(GAS)          1.0079E+00  4.2340E+03  6.5285E+01 08000000
  2 O    1/2_MOLE_O2(GAS)          1.5999E+01  4.3410E+03  1.0252E+02 08000000

 CURRENT NUMBER OF PHASE       2

 PHASE                          STATUS   SUBLATTICES
   1 GAS                        88200000     1
   2 H2O1_L                     82200000     1

 CURRENT NUMBER OF SPECIES     4

 SPECIES                                   STOICHIOMETRY
   1 H                           80800000   H
   2 H2O1                        00000000   H2O1
   3 O                           80800000   O
   4 VA                          81800000   VA

GES: @@ patch
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 H2O1_L                  ENTERED      0.000000E+00    0.000000E+00
 GAS                     ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY: c-st p h2o_l=e 0
   ... the command in full is CHANGE_STATUS
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/: CPS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT               STATUS    REF. STATE     T(K)           P(Pa)
 VA                      ENTERED   SER
 H                       ENTERED   SER
 O                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 H2O1_L                  ENTERED      0.000000E+00    0.000000E+00
 GAS                     ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 H    ENTERED    H2O1 ENTERED    O    ENTERED    VA   ENTERED
POLY: s-c t=380 p=1e5 n=100 ac(o)=1
   ... the command in full is SET_CONDITION
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0
POLY: 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 T=380, P=1E5, N=100, AC(O)=1
 DEGREES OF FREEDOM 0

 Temperature    380.00 K (   106.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.04643E+07,  Enthalpy -7.96861E+06,  Volume  1.05317E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 2.6556E-22 -1.5697E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                          Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00  Mole fractions:
```

```
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY: s-c p=none
   ... the command in full is SET_CONDITION
POLY: s-c s
   ... the command in full is SET_CONDITION
Value /6567.729231/: 6100
POLY: s-c t=350
   ... the command in full is SET_CONDITION
POLY: 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: l-e,,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: SUBDEMO

 Conditions:
 T=350, N=100, AC(O)=1, S=6100
 DEGREES OF FREEDOM 0

 Temperature    350.00 K (    76.85 C),  Pressure  4.130269E+04
 Number of moles of components  1.00000E+02,  Mass in grams  6.00493E+02
 Total Gibbs energy -1.03545E+07,  Enthalpy -8.21947E+06,  Volume  1.98337E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H                       6.6667E+01  6.6667E-01 6.6188E-24 -1.5532E+05 SER
 O                       3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

 GAS                         Status ENTERED     Driving force  0.0000E+00
 Moles 8.4450E+01, Mass 5.0711E+02, Volume fraction 1.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00

 H2O1_L                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.5550E+01, Mass 9.3379E+01, Volume fraction 0.0000E+00  Mole fractions:
 H  6.66667E-01  O  3.33333E-01
 Constitution:
 H2O1  1.00000E+00
POLY: @@ step in S with t=350
POLY: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: save tcex39d y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
...OK

 Phase Region from    6100.00     for:
     GAS
     H2O1_L
 Global test at  6.30000E+03 .... OK
 Global test at  6.55000E+03 .... OK
 Global check of removing phase at  6.71967E+03
 Calculated    27 equilibria

 Phase Region from    6719.67     for:
     GAS
 Global test at  6.90000E+03 .... OK
 Terminating at    7000.00
 Calculated    15 equilibria

 Phase Region from    6100.00     for:
     GAS
     H2O1_L
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: read,,,,
   ... the command in full is READ_WORKSPACES
POLY: s-c s=6000
   ... the command in full is SET_CONDITION
POLY: 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: @@ step in T with S=6000
POLY: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    350.000
...OK

 Phase Region from    350.000     for:
     GAS
     H2O1_L
 Global test at  3.70000E+02 .... OK
 Global test at  3.95000E+02 .... OK
 Global test at  4.20000E+02 .... OK
 Global test at  4.45000E+02 .... OK
 Terminating at    450.000
 Calculated    43 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: read,,,,
   ... the command in full is READ_WORKSPACES
POLY: s-c t=450
   ... the command in full is SET_CONDITION
POLY: 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
```

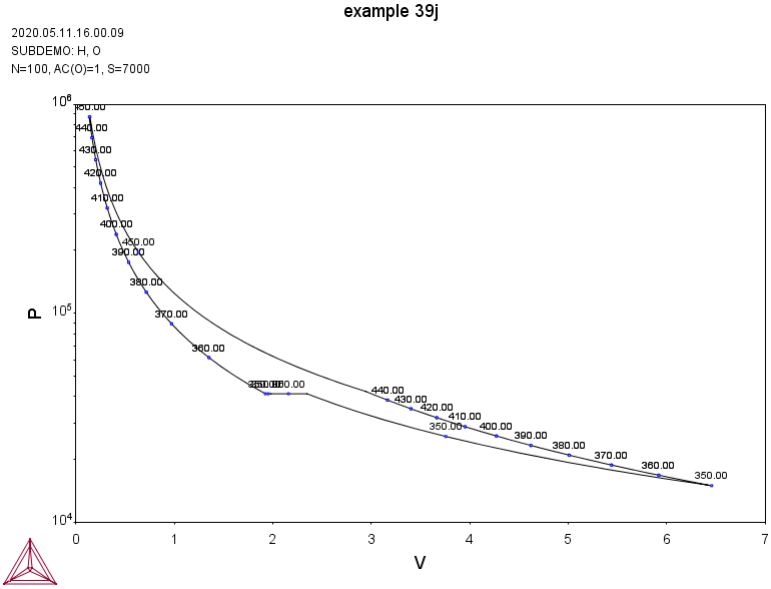
```
POLY: @@ Step in S with t=450
POLY: @@
POLY: s-a-v 1 s 6000 7000,,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    6100.00
...OK

 Phase Region from    6100.00     for:
     GAS
     H2O1_L
 Global check of removing phase at  6.16203E+03
 Calculated     5 equilibria

 Phase Region from    6162.03     for:
     GAS
 Global test at  6.35000E+03 .... OK
 Global test at  6.60000E+03 .... OK
 Global test at  6.85000E+03 .... OK
 Terminating at    7000.00
 Calculated    37 equilibria

 Phase Region from    6100.00     for:
     GAS
     H2O1_L
 Terminating at    6000.00
 Calculated     7 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: s-c s=7000
   ... the command in full is SET_CONDITION
POLY: 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: @@ Step in T with S=7000
POLY: s-a-v 1 t 350 450,,,
   ... the command in full is SET_AXIS_VARIABLE
POLY: step norm
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    450.000
...OK

 Phase Region from    450.000     for:
     GAS
 Global test at  4.30000E+02 .... OK
 Global test at  4.05000E+02 .... OK
 Global test at  3.80000E+02 .... OK
 Global test at  3.55000E+02 .... OK
 Terminating at    350.000
 Calculated    43 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex39\tcex39d.POLY3
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: @@ The cycle shows the constant pressure at phase transformation.
POST: s-p-f ##1,,,,,,,,,
   ... the command in full is SET_PLOT_FORMAT
 CURRENT DEVICE: TC-UNITE Driver
POST:
POST: @@ To get a better understanding of this process it is possible
POST: @@ to plot the cycle using any set of thermodynamic state
POST: @@ variables. From the pressure-volume-temperature diagram,
POST: @@ example 39g, youcan see the temperature variation on the
POST: @@ two adiabatical stages of the Carnot cycle.
POST: @@ The cycle shows the constant pressure at phase
POST: @@ transformation.
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 39h
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



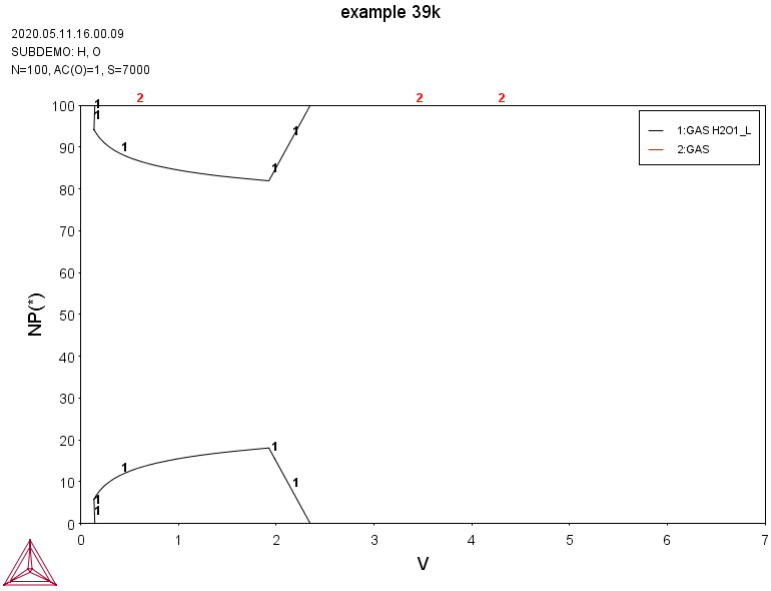

```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-tit example 39i
   ... the command in full is SET_TITLE
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



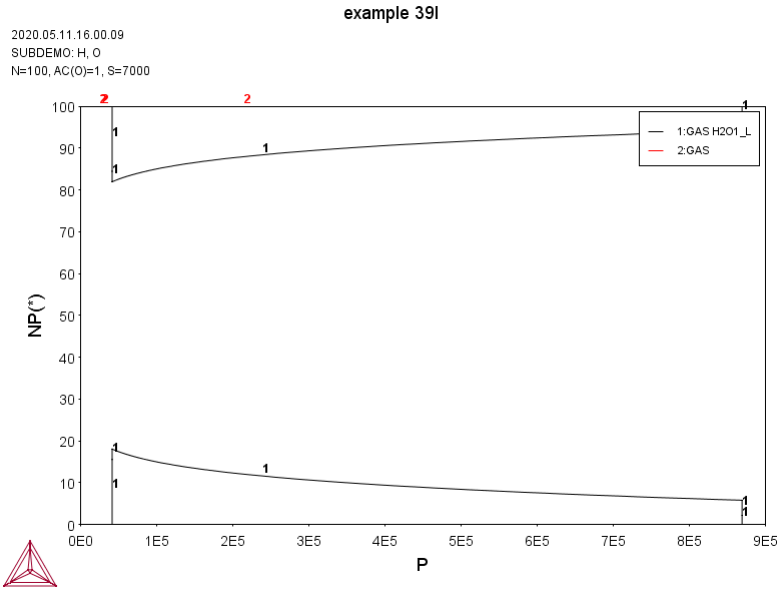

```
POST:
POST:Hit RETURN to continue
POST: s-d-a z t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab none
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39j
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



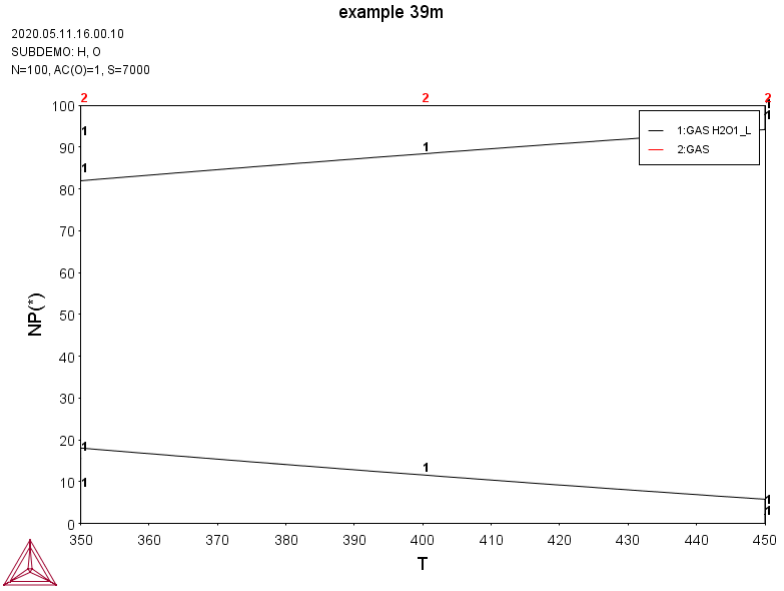

```
POST:
POST:Hit RETURN to continue
POST: @@ Another interesting aspect is it plots the amount of phases
POST: @@ versus volume. You can get information about both the kind
POST: @@ and amount of  phases that fill up a certain volume.
POST:
POST: s-d-a z none
   ... the command in full is SET_DIAGRAM_AXIS
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:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



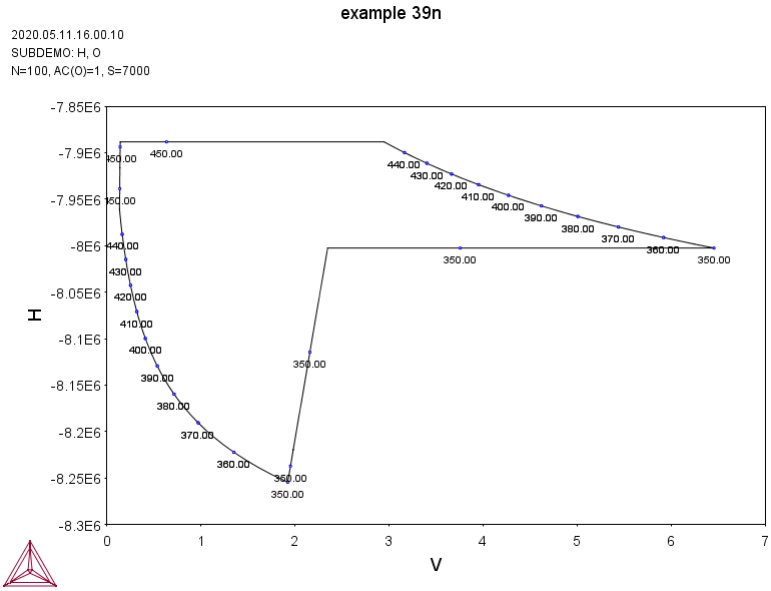

```
POST:
POST:Hit RETURN to continue
POST: @@ The next plot shows the amount of phases versus pressure. It
POST: @@ gives important information on the phase transformation
POST: @@ pressure and on the ratio between the two phases in
POST: @@ equilibrium at a certain pressure.
POST:
POST: s-d-a x p
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39l
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



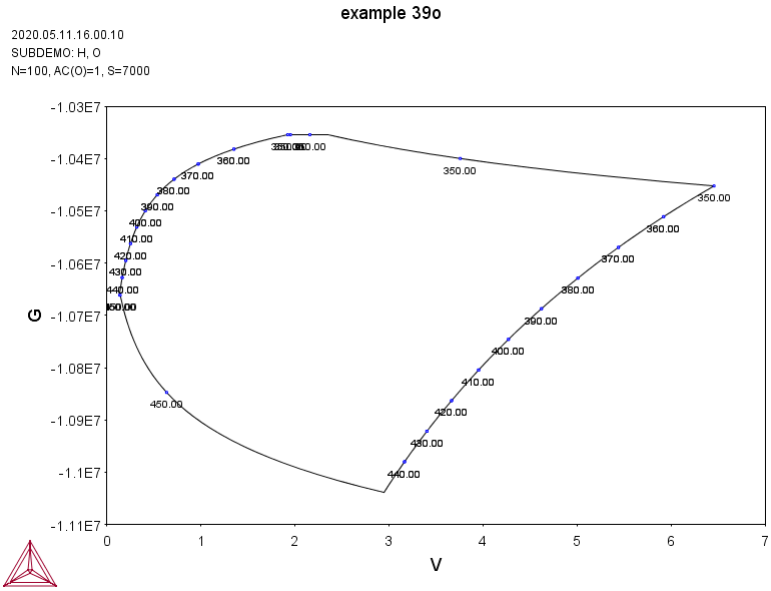

```
POST:
POST:Hit RETURN to continue
POST: @@ By ploting the amount of phases versus temperature,
POST: @@ example 39k, it is possible to know the phase transformation
POST: @@ temperature and the ratio between the two phases in
POST: @@ equilibrium at a certain temperature.
POST:
POST: s-d-a x t
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39m
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: @@ The enthalpy and Gibbs energy for the Carnot cycle could
POST: @@ also be ploted using the same calculation but a different
POST: @@ set for diagram axis. Note the important drop of the
POST: @@ enthalpy at the phase transformation point, example 39L.
POST:
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:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-d-a x v
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y g
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39o
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex40-TCEX40

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex40\TCEX40.TCM.test"
SYS: @@ POURBAIX module
SYS:
SYS: set-echo
SYS: set-ges-version 5
SYS: set-log TCEX40.LOG
Heading: Part 1 - Pourbaix Diagram Calculations with the advanced POURBAIX module
SYS:
SYS: @@ Delete both for Windows and Linux to be able to run macro twice without stumbling on existing EXP file
SYS:
SYS: @@ TCEX40: Thermo-Calc (Console Mode) Standard Example No 40
SYS: @@ ==========================================================
SYS: @@   Copyright: Thermo-Calc Software AB, Stockholm, Sweden
SYS: @@   Developer: Dr. Pingfang Shi, Thermo-Calc Software AB
SYS: @@   Date:      2014-05-18 (revision)
SYS: @@   Text updated July 2017 (AJW)
SYS:
SYS: @@ ==========================================================
SYS: @@ Example description:
SYS: @@ ==========================================================
SYS: @@ TCEX40 is the first in a series of examples to demonstrate
SYS: @@ the POURBAIX module calculations and plotting.
SYS: @@ - Uses Option 1: Start a new Pourbaix diagram calculation
SYS: @@ - Part 1 of a 6 part example.
SYS: @@ - Uses the TCS Public Aqueous Solution Database (PAQ2);
SYS: @@ - For the Fe-H2O-NaCl heterogeneous interaction system
SYS:
SYS: @@ The example automatically calculates and plots a Pourbaix
SYS: @@ diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at
SYS: @@ 25C and 1 bar. Other diagrams, along various phase
SYS: @@ boundaries for the same interactions resulting from the
SYS: @@ same Pourbaix module calculation, are also plotted.
SYS:
SYS: @@ ==========================================================
SYS: @@ Notes about the examples and the PAQ2 database:
SYS: @@ ==========================================================
SYS: @@ The so-called Pourbaix diagram is actually a phase diagram
SYS: @@ with independently-varied electropotential (Eh) and
SYS: @@ acidity (pH),for an heterogeneous interaction system at a
SYS: @@ certain bulk composition (that is by default always set as
SYS: @@ 1 kg of water  solving a specified amount of metals and
SYS: @@ other solutes), under defined temperature and pressure
SYS: @@ conditions.
SYS:
SYS: @@ This example uses Option 1 followed by a choice of a
SYS: @@ single database, i.e., retrieving data from the PAQ2
SYS: @@ database. For this and other Thermo-Calc simulations,
SYS: @@ it can also be done with the TDB-GES-POLY-POST routine,
SYS: @@ which is used in example TCEX53.
SYS:
SYS: @@ The PAQ2 database is specially designed for Pourbaix
SYS: @@ diagram calculations (i.e., Eh-pH plots). It contains an
SYS: @@ AQUEOUS solution phase and REF_ELECTRODE phase (as a
SYS: @@ reference for electron in aqueous electrolyte systems),
SYS: @@ as well as some data for various solid phases (solution
SYS: @@ or stoichiometric) and a gaseous mixture phase.
SYS:
SYS: @@ A POLY3 file (POURBAIX.POLY3) is automatically saved at the
SYS: @@ end of the calculation. The POURBAIX.POLY3 file can be used
SYS: @@ with the other options and examples:
SYS: @@   Option 2: to plot other property diagrams of the calculated
SYS: @@             interaction system. See TCEX40B.
SYS: @@   Option 3: to make another Pourbaix calculation of the same
SYS: @@             chemical system but under different P-T-X
SYS: @@             conditions. See TCEX40C.
SYS: @@   Option 4: to make a POLY3 STEPPING calculation of the same
SYS: @@             chemical system but varied with only one
SYS: @@             independent variable. See TCEX40D.
SYS:
SYS: @@ ** If you use the POLY3 file with the other examples it is
SYS: @@    important to make copies and rename these (for example
SYS: @@    TCEX40A.POLY3, TCEX40B.POLY3, etc.). This must be done
SYS: @@    outside of the Thermo-Calc software and after the TCEX40
SYS: @@    calculation and plotting is complete. This is so that the
SYS: @@    required POLY3 file structure is not lost.
SYS:
SYS: @@ ** A more advanced version of 40 and 40A can be found in
SYS: @@    TCEX40E, which also uses Option 1 but with multiple
SYS: @@    databases. However, licenses are required for three
SYS: @@    commercial Thermo-Calc databases. See the online help
SYS: @@    and the 40E macro text.
SYS: @@ ----------------------------------------------------------
SYS:
SYS: @@... Now, let's start using the advanced POURBAIX module:
SYS: @@
SYS: go pour
   ... the command in full is GOTO_MODULE

                 WELCOME TO THE POURBAIX MODULE
                 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!
          for Quick Calculations of Pourbaix Diagrams
          ===========================================

                   Pingfang Shi and Bo Sundman
```

Thermo-Calc Software AB
Norra Stationsgatan 93
SE-113 47 Stockholm, Sweden

(Version 7.0, Mar. 2014)

Need any instruction on the POURBAIX module? /N/: ?

IMPORTANT NOTES for Calculating a POURBAIX Diagram:
---

1) The so-called Pourbaix diagram is actually a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (Eh, as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modelled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).
2) One must have at least a database containing an AQUEOUS solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc database spectrum, or be chosen from an appropriate USER-specified database (it must be in the Thermo-Calc TDB format).
3) Due to the restrictions of aqueous solution model used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ) or AQS (PAQS) for AQUEOUS solution phase. Among others, one should keep in mind the following regulations:
   * The ELECTRON is defined as an special element (ZE) and as the only constituent in its reference phase REFERENCE_ELECTRODE (for determining the electro-potential that is defined as Eh with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;
   * The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;
   * The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.
4) Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H2O1, O2 and H2; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!
5) All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a GASeous mixture phase, a REF_ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above). Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the TCAQ or AQS as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended). Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAl, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for GASeous mixture phase and for varous solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.
6) The current advanced POURBAIX-Module has been designed and developed in an efficient and effective way that it only requires the user to just answer some simple and necessary questions, rather than to go through basic modules (i.e., TDB, GES5, POLY3 and POST) and type the ordinary command-lines. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.
7) The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-PLOY3-POST calculation.

Enforce a PAUSE after plotting when running a MACRO? /N/: ?

Whenever running a Thermo-Calc MACRO (TCM) file, you may prefer to have a PAUSE after a specific diagram has been plotted on SCREEN, for the multiple purposes of efficiently and easily manipulating the plotted diagram directly on the traditional TC-Graph window or Java-based TC-UNITE window,

```
    such as:
      * Printing it (of EMF/PS format) on connected printer(s);
      * Converting it (of EMF format) to (PDF) graphical files;
      * Saving it as an EMF graphical file;
      * Dumping it as a PNG or BMP graphical file;
      * Setting background colour for the current diagram
          and for all the sequential plots;
      * Setting default font/size for all the sequential plots;
      * Changing plotting Layers for all the sequential plots.

    If no PAUSE is enforced, the POURBAIX Module will be going
    through all the sequential command-lines (answers) in the
    same POURBAIX session or till the SET_INTERACTIVE_MODE line
    in the MACRO file has been reached.

    ---------------------------------------------------------
    ** By Y(y), a PAUSE is always enforced after each diagram;
    ** By N(n), no PAUSE will be enforced at any point at all.
    ---------------------------------------------------------
    Please then press <RETURN> at the PAUSE for continuation!
```

Enforce a PAUSE after plotting when running a MACRO? /N/: y

```
    ---------------------------------------------------------
   |                                                         |
   |  1. Start a completely new POURBAIX diagram calculation  |
   |  2. Open an old file & plot other property diagrams      |
   |  3. Open an old file & make another POURBAIX calculation |
   |  4. Open an old file & make another STEPPING calculation |
   |                                                         |
    ---------------------------------------------------------
```

Select option /1/: ?

```
   One of the four options (1/2/3/4) should be entered here:

    1 -- Make a completely new POURBAIX diagram calculation
           and automatically plot a pH-Eh diagram.
              i.e., define a new chemical system;
                    specify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.

    2 -- Open an existing POLY3 file created by POURBAIX Module
            (from a previous POURBAIX calculation Option 1 or 3
              or  a previous STEPPING calculation Option 4),
           and just selectively plot other property diagrams.
              i.e., open the old GES and POLY3 workspaces;
                    plot pH-Eh or various property diagrams.

    3 -- Open an existing POLY3 file created by POURBAIX Module
           and make another POURBAIX diagram calculation.
              i.e., open the old GES and POLY3 workspaces;
                    adopt the defined chemical system;
                    modify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.

    4 -- Open an existing POLY3 file created by POURBAIX Module
            (from a previous POURBAIX calculation Option 1 or 3
              or  a previous STEPPING calculation Option 4),
           and make a normal STEPPING calculation.
              i.e., open the old GES and POLY3 workspaces;
                    adopt the defined chemical system;
                    specify one of the T-P-X conditions
                             as the stepping variable;
                    calculate the initial equilibria;
                    perform the stepping calculation;
                    plot various property diagrams.
```

Select option /1/: 1

```
    1 -- Make a completely new POURBAIX diagram calculation
           and automatically plot a pH-Eh diagram.
              i.e., define a new chemical system;
                    specify the T-P-X conditions;
                    calculate the initial equilibria;
                    perform the pH-Eh mapping calculation;
                    plot pH-Eh & various property diagrams.
```

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: ?

```
    You may optionally choose to ignore the GAS mixture phase
    on a calculated/plotted Pourbaix diagram. However, such a
    plot is actually not a complete Pourbaix diagram, due to
    that the thermodynamically-stable phase boundaries between
    the AQUEOUS solution phase and GAS mixture phase will not
    be calculated at all.

    ---------------------------------------------------------
    ** By Y(y), GAS mixture phase shall be always considered;
    ** By N(n), GAS mixture phase will be completely ignored.
    ---------------------------------------------------------
```

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: Y

Use single database? /Y/: Y
Combined Database: /PAQ2/: PAQ2

```
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Public Aqueous Soln (SIT) TDB v2.4

 H                       O                       ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                DIAMOND_A4              FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                CUB_A13                 CHI_A12
 FE4N                    FECN_CHI  REJECTED
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 PI  REJECTED
 FE3C                    NI3C                    CR3C2
```

```
 CR7C3                    CR23C6  REJECTED
 COCO3                    FECO3                    NAHCO3
 NA2CO3                   NA2CO3_S2                NICO3
 CRC6O6  REJECTED
 CO3N                     CRN                      CR2N
 FE2N                     NI3N  REJECTED
 NANO2                    NANO2_S2                 NANO3
   REJECTED
 COCL2                    CRCL2                    CRCL3
 FECL2                    FECL3                    NICL2
   REJECTED
 FECLO                    NACLO4                   NACLO4_S2
   REJECTED


 DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION:
 ==========================================================
 Normally a POURBAIX diagram and related equilibrium property
 in a heterogeneous interaction system are calculated under a
 certain bulk composition which is usually 1 kg of water with
 defined amounts of dissolving solute substances. The solutes
 may either be completely dissolved into the aqueous solution,
 or be partially dissolved and simultaneously form some solid
 phases.

 CHEMICAL SYSTEM (ELEMENTS):
    Default defined elements  (solvent  H2O):     H  &  O
            and specially assigned ZE(electron) & VA(vacancy).
    Prompt specified elements (solutes  ELEM):
            Fe  Ni  Co  Cr  C   N   S   Na  Cl
 INITIAL BULK COMPOSITION:
    Default defined composition  (solvent):    1.0 kg of H2O
    Prompt specified composition (solutes):    x mole of ELEM
 ----------------------------------------------------------
 Notes: For accepting a default value, just RETURN at prompt;
        For changing to a specific value, enter it at prompt.

 ==========================================================
 IMPORTANT NOTE for Entering Solutes in Chemical Formulas:
   First element letter in UPPER case, and second lower case!
     such as  NaCl  CO2  CoCl3  Fe0.93S  NaSO4-1  H2SO4
 ----------------------------------------------------------
   Mass of Water (weight) = 1 kg

   First solute: Fe
     Molality of Fe [mol/kg] /.001/: .001
   Second solute: NaCl .1
   Next solute:

 ---------------------------------------------------------
 Defined chemical system and initial bulk composition:
    Note: Solutes have been split up into chemical elements
          and their mole numbers. If confirmed, the POURBAIX
          Module will, in further steps, count the initial
          bulk composition in terms of chemical elements.
 ---------------------------------------------------------
         H2O           1.00000000       kg
         ZE           (specially assigned)
          FE          0.1000000000E-02  mole
          CL          0.1000000000E+00  mole
          NA          0.1000000000E+00  mole

Confirm defined system and initial bulk composition? /Y/: Y


RETRIEVE THERMODYNAMIC DATA FROM THE DATABASE:  PAQ2

 H                        O                        ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                 DIAMOND_A4               FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                 CUB_A13                  CHI_A12
 FE4N                     FECN_CHI  REJECTED
 CEMENTITE                M23C6                    M7C3
 M5C2                     M3C2                     KSI_CARBIDE
 PI  REJECTED
 FE3C                     NI3C                     CR3C2
 CR7C3                    CR23C6  REJECTED
 COCO3                    FECO3                    NAHCO3
 NA2CO3                   NA2CO3_S2                NICO3
 CRC6O6  REJECTED
 CO3N                     CRN                      CR2N
 FE2N                     NI3N  REJECTED
 NANO2                    NANO2_S2                 NANO3
   REJECTED
 COCL2                    CRCL2                    CRCL3
 FECL2                    FECL3                    NICL2
   REJECTED
 FECLO                    NACLO4                   NACLO4_S2
   REJECTED
 REINITIATING GES .....
 FE  DEFINED
 CL  DEFINED
 NA  DEFINED
 /-  DEFINED


 This database has following phases for the defined system

 AQUEOUS:A                 REF_ELECTRODE            GAS:G
 FCC_A1                    BCC_A2                   HCP_A3
 HALITE                    WUSTITE                  MAGNETITE
 HEMATITE                  FE2O3_GAMMA              FEO2H2
 FEO3H3                    FEOOH                    FE2O2O2H2
 NAO2                      NA2O                     NA2O_S2
 NA2O_S3                   NA2O2                    NA2O2_S2
 NAOH                      NAOH_S2                  NA2FEO2
Reject phase(s) /NONE/: HCP_A3
 HCP_A3  REJECTED
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

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

```
    The following phases are retained in this system:

 AQUEOUS:A                 REF_ELECTRODE             GAS:G
 FCC_A1                    BCC_A2                    HALITE
 WUSTITE                   MAGNETITE                 HEMATITE
 FE2O3_GAMMA               FEO2H2                    FEO3H3
 FEOOH                     FE2O2O2H2                 NAO2
 NA2O                      NA2O_S2                   NA2O_S3
 NA2O2                     NA2O2_S2                  NAOH
 NAOH_S2                   NA2FEO2

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

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

 List of references for assessed data

  'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
      -Cl system.'
  'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
      -Cr-Na-Ni-C-H-O-N-S-Cl system.'
  'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
      -Na-Ni-C-H-O-N-S-Cl system.'
  'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
      only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
      from TCAQ2 which covers totally 83 elements and contains many more
      aqueous solution species.'
 -OK-
Should any phase have a miscibility gap check? /N/: N

      ...... Reinitializing POLY3 workspaces ......

Enforce Global Minimization Technique in calculations? /N/: N

Save all functions, variables and tables in POLY3 file? /Y/: Y

Set numerical limits? /N/: N


SET CALCULATING PARAMETERS:
 Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
 Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead

 List of Default and Pre-defined Calculation Conditions:
 ---------------------------------------------------------------
  Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole
 ---------------------------------------------------------------
 T=298.15, P=1E5, B(H2O)=1000, N(H+1)=0, N(ZE)=0, N(CL)=0.1, N(FE)=1E-3,
    N(NA)=0.1
 DEGREES OF FREEDOM 0

Confirm defined conditions? /Y/: Y

 Calculating start points; please be patient!


LIST THE FIRST DEFAULT STARTING EQUILIBRIUM POINT:

 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 T=298.15, P=1E5, B(H2O)=1000, N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.1181, MUR(ZE)=100
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.57094E+01,  Mass in grams  1.00590E+03
 Total Gibbs energy -1.70696E+07,  Enthalpy -1.59069E+07,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 CL                      1.0000E-01  1.7950E-03 1.4499E-30 -1.7032E+05 SER
 FE                      1.0000E-03  1.7950E-05 4.6321E-26 -1.4461E+05 SER
 H+1                    -3.0000E-03 -5.3851E-05 1.0000E-07 -3.9956E+04 SER
 NA                      1.0000E-01  1.7950E-03 1.7205E-50 -2.8406E+05 SER
 H2O                     5.5508E+01  9.9639E-01 9.9593E-01 -1.0110E+01 AQUEOUS
 ZE                      3.0000E-03  5.3851E-05 1.0412E+00  1.0000E+02 REF_ELEC

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5707E+01, Mass 1.0058E+03, Volume fraction 0.0000E+00  Mole fractions:
 H2O  9.96410E-01  NA   1.79511E-03  FE   1.08146E-11
 CL   1.79511E-03  ZE   2.03382E-11  H+1 -1.36468E-11
 Constitution:           SiteFraction    Molality      Activity    log10Act
 H2O                      9.96410E-01   5.55084E+01   9.96012E-01    -0.0017
 CL-1                     1.79511E-03   1.00003E-01   7.76756E-02    -1.1097
 NA+1                     1.79511E-03   1.00003E-01   7.76756E-02    -1.1097
 OH-1                     2.31689E-09   1.29070E-07   1.00218E-07    -6.9991
 H+1                      2.30788E-09   1.28568E-07   1.00000E-07    -7.0000
 FE+2                     6.21477E-12   3.46215E-10   1.26203E-10    -9.8989
 FEOH+1                   4.59380E-12   2.55913E-10   1.99003E-10    -9.7011
 O3                       1.00000E-15   0.00000E+00   2.6033E-113  -112.5845
 H2O2                     1.00000E-15   0.00000E+00   3.63324E-46   -45.4397
 HCLO                     1.00000E-15   0.00000E+00   3.55905E-45   -44.4487
 H2                       1.00000E-15   0.00000E+00   5.46000E-18   -17.2628
 HCLO2                    1.00000E-15   0.00000E+00   1.38939E-87   -86.8572
 FEOH+2                   1.00000E-15   0.00000E+00   9.27035E-19   -18.0329
 HO2-1                    1.00000E-15   0.00000E+00   7.68880E-51   -50.1141
 FEO3H3-1                 1.00000E-15   0.00000E+00   1.69673E-51   -50.7704
 FECL+2                   1.00000E-15   0.00000E+00   3.39801E-23   -22.4688
 FE2O2H2+4                1.00000E-15   0.00000E+00   3.71405E-35   -34.4302
 FE+3                     1.00000E-15   0.00000E+00   1.53892E-23   -22.8128
 O2                       1.00000E-15   0.00000E+00   2.54948E-58   -57.5935
 CLO4-1                   1.00000E-15   0.00000E+00   8.8489E-133  -132.0531
 CLO3-1                   1.00000E-15   0.00000E+00   1.5694E-105  -104.8043
 CLO2-1                   1.00000E-15   0.00000E+00   1.45414E-82   -81.8374
 CLO2                     1.00000E-15   0.00000E+00   1.6417E-100   -99.7847
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 CLO-1                    1.00000E-15   0.00000E+00   7.71560E-46   -45.1126
 CL2                      1.00000E-15   0.00000E+00   5.82418E-50   -49.2348
 Solution Properties:   pH =   7.0000    Eh =    0.0010 V     I =   0.1000
                        pe =   0.0175    Ah =    0.1000 kJ   m* =   0.2000
                        Aw =   0.9960    Os =    1.1089     pKw =  13.9973
                        At1= 1.0000E-15  At2= 1.2907E-07 (equiv_mol/kg_H2O)

 HEMATITE                     Status ENTERED     Driving force  0.0000E+00
 Moles 2.5000E-03, Mass 7.9846E-02, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.20000E+00  FE   4.00000E-01  NA   0.00000E+00
 H2O  6.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00
 Constitution:
 FE2O3  1.00000E+00

LIST THE DEFINED SYMBOLS:
 DEFINED CONSTANTS
    TSLIMIT0=99, AH2O=55.508435, WH2O=1.80152E-2, RNL=2.3025851, R=8.31451,
       RNF=96485.309
 DEFINED FUNCTIONS AND VARIABLES%
    TC%=T-273.15
    PBAR%=P*1E-05
    PKB%=P*1E-08
    RT%=R*T
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
    YH2O=Y(AQUEOUS,H2O)
    ACRH2O=ACR(H2O,AQUEOUS)
    RCH2O=ACR(H2O,AQUEOUS)
    MLH2O=AH2O
    ACTW=ACRH2O
    OSMC=-YH2O/ (1-YH2O )* LOG(ACRH2O )
    TMI= (1-YH2O )*AH2O/YH2O
    AHZE=MUR(ZE)/1000
    PEZE=MUR(ZE)/ (RNL*RT )
    AI1=ACR(CL-1,AQUEOUS)*AH2O
    RC1=ACR(CL-1,AQUEOUS)*YH2O/Y(AQUEOUS,CL-1)
    ML1=Y(AQUEOUS,CL-1)*AH2O/YH2O
    AI2=ACR(CL2,AQUEOUS)*AH2O
    RC2=ACR(CL2,AQUEOUS)*YH2O/Y(AQUEOUS,CL2)
    ML2=Y(AQUEOUS,CL2)*AH2O/YH2O
    AI3=ACR(CLO-1,AQUEOUS)*AH2O
    RC3=ACR(CLO-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO-1)
    ML3=Y(AQUEOUS,CLO-1)*AH2O/YH2O
    AI4=ACR(CLO2,AQUEOUS)*AH2O
    RC4=ACR(CLO2,AQUEOUS)*YH2O/Y(AQUEOUS,CLO2)
    ML4=Y(AQUEOUS,CLO2)*AH2O/YH2O
    AI5=ACR(CLO2-1,AQUEOUS)*AH2O
    RC5=ACR(CLO2-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO2-1)
    ML5=Y(AQUEOUS,CLO2-1)*AH2O/YH2O
    AI6=ACR(CLO3-1,AQUEOUS)*AH2O
    RC6=ACR(CLO3-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO3-1)
    ML6=Y(AQUEOUS,CLO3-1)*AH2O/YH2O
    AI7=ACR(CLO4-1,AQUEOUS)*AH2O
    RC7=ACR(CLO4-1,AQUEOUS)*YH2O/Y(AQUEOUS,CLO4-1)
    ML7=Y(AQUEOUS,CLO4-1)*AH2O/YH2O
    AI8=ACR(FE+2,AQUEOUS)*AH2O
    RC8=ACR(FE+2,AQUEOUS)*YH2O/Y(AQUEOUS,FE+2)
    ML8=Y(AQUEOUS,FE+2)*AH2O/YH2O
    AI9=ACR(FE+3,AQUEOUS)*AH2O
    RC9=ACR(FE+3,AQUEOUS)*YH2O/Y(AQUEOUS,FE+3)
    ML9=Y(AQUEOUS,FE+3)*AH2O/YH2O
    AI10=ACR(FE2O2H2+4,AQUEOUS)*AH2O
    RC10=ACR(FE2O2H2+4,AQUEOUS)*YH2O/Y(AQUEOUS,FE2O2H2+4)
    ML10=Y(AQUEOUS,FE2O2H2+4)*AH2O/YH2O
    AI11=ACR(FECL+2,AQUEOUS)*AH2O
    RC11=ACR(FECL+2,AQUEOUS)*YH2O/Y(AQUEOUS,FECL+2)
    ML11=Y(AQUEOUS,FECL+2)*AH2O/YH2O
    AI12=ACR(FEO3H3-1,AQUEOUS)*AH2O
    RC12=ACR(FEO3H3-1,AQUEOUS)*YH2O/Y(AQUEOUS,FEO3H3-1)
    ML12=Y(AQUEOUS,FEO3H3-1)*AH2O/YH2O
    AI13=ACR(FEOH+1,AQUEOUS)*AH2O
    RC13=ACR(FEOH+1,AQUEOUS)*YH2O/Y(AQUEOUS,FEOH+1)
    ML13=Y(AQUEOUS,FEOH+1)*AH2O/YH2O
    AI14=ACR(FEOH+2,AQUEOUS)*AH2O
    RC14=ACR(FEOH+2,AQUEOUS)*YH2O/Y(AQUEOUS,FEOH+2)
    ML14=Y(AQUEOUS,FEOH+2)*AH2O/YH2O
    AI15=ACR(H+1,AQUEOUS)*AH2O
    RC15=ACR(H+1,AQUEOUS)*YH2O/Y(AQUEOUS,H+1)
    ML15=Y(AQUEOUS,H+1)*AH2O/YH2O
    AI16=ACR(H2,AQUEOUS)*AH2O
    RC16=ACR(H2,AQUEOUS)*YH2O/Y(AQUEOUS,H2)
    ML16=Y(AQUEOUS,H2)*AH2O/YH2O
    AI17=ACR(H2O,AQUEOUS)
    RC17=ACR(H2O,AQUEOUS)/Y(AQUEOUS,H2O)
    ML17=Y(AQUEOUS,H2O)*AH2O/YH2O
    AI18=ACR(H2O2,AQUEOUS)*AH2O
    RC18=ACR(H2O2,AQUEOUS)*YH2O/Y(AQUEOUS,H2O2)
    ML18=Y(AQUEOUS,H2O2)*AH2O/YH2O
    AI19=ACR(HCLO,AQUEOUS)*AH2O
    RC19=ACR(HCLO,AQUEOUS)*YH2O/Y(AQUEOUS,HCLO)
    ML19=Y(AQUEOUS,HCLO)*AH2O/YH2O
    AI20=ACR(HCLO2,AQUEOUS)*AH2O
    RC20=ACR(HCLO2,AQUEOUS)*YH2O/Y(AQUEOUS,HCLO2)
    ML20=Y(AQUEOUS,HCLO2)*AH2O/YH2O
    AI21=ACR(HO2-1,AQUEOUS)*AH2O
    RC21=ACR(HO2-1,AQUEOUS)*YH2O/Y(AQUEOUS,HO2-1)
    ML21=Y(AQUEOUS,HO2-1)*AH2O/YH2O
    AI22=ACR(NA+1,AQUEOUS)*AH2O
    RC22=ACR(NA+1,AQUEOUS)*YH2O/Y(AQUEOUS,NA+1)
    ML22=Y(AQUEOUS,NA+1)*AH2O/YH2O
    AI23=ACR(O2,AQUEOUS)*AH2O
    RC23=ACR(O2,AQUEOUS)*YH2O/Y(AQUEOUS,O2)
    ML23=Y(AQUEOUS,O2)*AH2O/YH2O
    AI24=ACR(O3,AQUEOUS)*AH2O
    RC24=ACR(O3,AQUEOUS)*YH2O/Y(AQUEOUS,O3)
    ML24=Y(AQUEOUS,O3)*AH2O/YH2O
    AI25=ACR(OH-1,AQUEOUS)*AH2O
    RC25=ACR(OH-1,AQUEOUS)*YH2O/Y(AQUEOUS,OH-1)
    ML25=Y(AQUEOUS,OH-1)*AH2O/YH2O
    IS1=.5*ML1+.5*ML3+.5*ML5
    IS2=.5*ML6+.5*ML7+.5*ML8*2**2
    IS3=.5*ML9*3**2+.5*ML10*4**2+.5*ML11*2**2
    IS4=.5*ML12+.5*ML13+.5*ML14*2**2
    IS5=.5*ML15+.5*ML21+.5*ML22
    ISTR=1*IS1+1*IS2+1*IS3+1*IS4+1*IS5
    RLOGH= LOG10(ACR(H+1,AQUEOUS)*AH2O )
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    RLOGOH= LOG10(ACR(OH-1,AQUEOUS)*AH2O )
    RLOGH2O= LOG10(ACRH2O )
 DEFINED TABLES
    GPT=T, P, PH, EH, ISTR
    SFT=Y(AQUEOUS,CL-1), Y(AQUEOUS,CL2), Y(AQUEOUS,CLO-1), Y(AQUEOUS,CLO2),
       Y(AQUEOUS,CLO2-1), Y(AQUEOUS,CLO3-1), Y(AQUEOUS,CLO4-1),
       Y(AQUEOUS,FE+2), Y(AQUEOUS,FE+3), Y(AQUEOUS,FE2O2H2+4),
       Y(AQUEOUS,FECL+2), Y(AQUEOUS,FEO3H3-1), Y(AQUEOUS,FEOH+1),
       Y(AQUEOUS,FEOH+2), Y(AQUEOUS,H+1), Y(AQUEOUS,H2), Y(AQUEOUS,H2O),
       Y(AQUEOUS,H2O2), Y(AQUEOUS,HCLO), Y(AQUEOUS,HCLO2), Y(AQUEOUS,HO2-1),
       Y(AQUEOUS,NA+1), Y(AQUEOUS,O2), Y(AQUEOUS,O3), Y(AQUEOUS,OH-1), PH, EH
    AYT=AC(CL-1,AQUEOUS), AC(CL2,AQUEOUS), AC(CLO-1,AQUEOUS),
       AC(CLO2,AQUEOUS), AC(CLO2-1,AQUEOUS), AC(CLO3-1,AQUEOUS),
       AC(CLO4-1,AQUEOUS), AC(FE+2,AQUEOUS), AC(FE+3,AQUEOUS),
       AC(FE2O2H2+4,AQUEOUS), AC(FECL+2,AQUEOUS), AC(FEO3H3-1,AQUEOUS),
       AC(FEOH+1,AQUEOUS), AC(FEOH+2,AQUEOUS), AC(H+1,AQUEOUS),
       AC(H2,AQUEOUS), AC(H2O,AQUEOUS), AC(H2O2,AQUEOUS), AC(HCLO,AQUEOUS),
       AC(HCLO2,AQUEOUS), AC(HO2-1,AQUEOUS), AC(NA+1,AQUEOUS), AC(O2,AQUEOUS),
       AC(O3,AQUEOUS), AC(OH-1,AQUEOUS), PH, EH
    ART=ACR(CL-1,AQUEOUS), ACR(CL2,AQUEOUS), ACR(CLO-1,AQUEOUS),
       ACR(CLO2,AQUEOUS), ACR(CLO2-1,AQUEOUS), ACR(CLO3-1,AQUEOUS),
       ACR(CLO4-1,AQUEOUS), ACR(FE+2,AQUEOUS), ACR(FE+3,AQUEOUS),
       ACR(FE2O2H2+4,AQUEOUS), ACR(FECL+2,AQUEOUS), ACR(FEO3H3-1,AQUEOUS),
       ACR(FEOH+1,AQUEOUS), ACR(FEOH+2,AQUEOUS), ACR(H+1,AQUEOUS),
       ACR(H2,AQUEOUS), ACR(H2O,AQUEOUS), ACR(H2O2,AQUEOUS),
       ACR(HCLO,AQUEOUS), ACR(HCLO2,AQUEOUS), ACR(HO2-1,AQUEOUS),
       ACR(NA+1,AQUEOUS), ACR(O2,AQUEOUS), ACR(O3,AQUEOUS), ACR(OH-1,AQUEOUS),
       PH, EH
    AIT=AI1, AI2, AI3, AI4, AI5, AI6, AI7, AI8, AI9, AI10, AI11, AI12, AI13,
       AI14, AI15, AI16, AI17, AI18, AI19, AI20, AI21, AI22, AI23, AI24, AI25,
       PH, EH
    RCT=RC1, RC2, RC3, RC4, RC5, RC6, RC7, RC8, RC9, RC10, RC11, RC12, RC13,
       RC14, RC15, RC16, RC17, RC18, RC19, RC20, RC21, RC22, RC23, RC24, RC25,
       PH, EH
    MLT=ML1, ML2, ML3, ML4, ML5, ML6, ML7, ML8, ML9, ML10, ML11, ML12, ML13,
       ML14, ML15, ML16, ML18, ML19, ML20, ML21, ML22, ML23, ML24, ML25, ISTR,
       PH, EH

 IMPORTANT FACTS:
     The default definitions of the Eh and pH quantities in the
       advanced POURBAIX-Module (and in the ordinary TDB-GES-POLY
       calculation routines) should ALWAYS be as below:
         Eh = MUR(ZE)/RNF
         pH = -log10[AI(H+1,AQUEOUS)]
            = -log10[ACR(H+1,AQUEOUS)*AH2O]
       where RNF is the Faraday constant (96485.309 C/mol),
       and AH2O is the molecular weight of H2O (55.508435 g).
       MUR(ZE) is the electrochemical potential (ECP; in the
       unit of J/mol; w.r.t. the standard hydrogen electrode).
       ACR(H+1,AQUEOUS) is the site-fraction-based activity of
       the H+1 aqueous species in AQUEOUS solution phase, but
       AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH2O] is
       the molality-based activity of the H+1 aqueous species
       that should be used for defining the pH quantity.

     Within an aqueous-bearing heterogeneous interaction system,
       the fundamental system-components must be H2O, H+1 and ZE,
       which are corresponding to the basic elements O & H and
       the hypothetical electron (ZE) in the aqueous solution
       phase. For the additional chemical elements in the system,
       their corresponding system-components shall be defined as
       in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S)
       or (for some) in their molecular forms (e.g., NaCl, H2S).
       The reference state for the H2O component must always be
       defined as the solvent species H2O in the AQUEOUS solution
       phase under the current temperature (*) and 100000 Pascal
       (i.e., 1 bar). The reference states for the H+1 and ZE
       components are by default set as their SER.

     Various conventional properties of aqueous solute species I
       are converted in the following manners:
         ML = Y(AQUEOUS,I)*AH2O/YH2O
         RC = ACR(I,AQUEOUS)*YH2O/Y(AQUEOUS,I)
         AI = RC*ML
            = ACR(I,AQUEOUS)*AH2O
       where YH2O [i.e., Y(AQUEOUS,H2O)] and Y(AQUEOUS,I) are
       the site-fractions of solvent H2O and solute species I.

LIST THE DEFINED AXIS-VARIABLES:

  Axis No 1: LNACR(H+1)            Min: -34.532608Max: 2.3025851 Inc: 0.8
  Axis No 2: MUR(ZE)               Min: -150000   Max: 200000    Inc: 7718.85

     NOTE: The default settings (listed above) for two mapping
           variables [in terms of lnACR(H+1) and MUR(ZE), and
           their minimum/maximum values and increment steps]
           are covering the following pH-Eh ranges/steps:
             pH:  0.00 -> 14.00, at a step of 0.35
             Eh: -1.55 ->  2.07, at a step of 0.08 [V]

           The maximum pH limit has been calculated precisely
           and determined automatically by the POURBAIX-Module,
           as a function of the temperature-pressure conditions
           and initial bulk compositions of the current defined
           interaction system.

Accept the default settings for two mapping variables? /Y/: Y


LIST ALL THE INITIAL EQUILIBRIA FOR MAPPING:

 No 1  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 2  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 3  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 4  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=100.
 No 5  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=-28400
 No 6  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=-28400
 No 7  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=-28400
 No 8  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
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    LNACR(H+1)=-16.118096, MUR(ZE)=-28400
 No 9  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
 No 10 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
 No 11 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
 No 12 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
 No 13 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 14 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 15 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 16 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-9.2103404, MUR(ZE)=86837
 No 17 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=66000.
 No 18 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=66000.
 No 19 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=66000.
 No 20 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.118096, MUR(ZE)=66000.


 MAP THE POURBAIX DIAGRAM:
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12
 Generating start point  13
 Generating start point  14
 Generating start point  15
 Generating start point  16
 Generating start point  17
 Generating start point  18
 Generating start point  19
 Generating start point  20
 Working hard
 Generating start point  21
 Generating start point  22
 Generating start point  23
 Generating start point  24
 Generating start point  25
 Generating start point  26
 Generating start point  27
 Generating start point  28
 Generating start point  29
 Generating start point  30
 Working hard
 Generating start point  31
 Generating start point  32
 Generating start point  33
 Generating start point  34
 Generating start point  35
 Generating start point  36
 Generating start point  37
 Generating start point  38
 Generating start point  39
 Generating start point  40
 Working hard
 Working hard
 Generating start point  41
 Generating start point  42
 Generating start point  43
 Generating start point  44
 Generating start point  45
 Generating start point  46
 Generating start point  47
 Generating start point  48

 Phase region boundary   1 at:  -1.612E+01  7.911E+04
     GAS
     AQUEOUS
  ** HALITE
     HEMATITE
 Calculated..                      25 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:  -3.453E+01  3.383E+04
     GAS
     AQUEOUS
  ** HALITE
     HEMATITE
 Calculated.                      42 equilibria

 Phase region boundary   3 at:  -2.296E+00  1.134E+05
     GAS
     AQUEOUS
  ** HALITE
  ** HEMATITE

 Phase region boundary   4 at:  -2.296E+00  1.134E+05
     GAS
     AQUEOUS
  ** HALITE
 Calculated                      33 equilibria
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```
Phase region boundary   5 at:  -2.296E+00  1.134E+05
    GAS
    AQUEOUS
 ** HEMATITE
Calculated                      5 equilibria

Phase region boundary   6 at:  -2.296E+00  1.134E+05
    GAS
    AQUEOUS
    HALITE
 ** HEMATITE
Calculated                     31 equilibria

Phase region boundary   7 at:  -1.612E+01  7.911E+04
    GAS
    AQUEOUS
 ** HALITE
    HEMATITE
Calculated.                     19 equilibria
Terminating at known equilibrium

Phase region boundary   8 at:  -1.612E+01  7.817E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     26 equilibria
Terminating at axis limit.

Phase region boundary   9 at:  -3.453E+01  3.296E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     43 equilibria

Phase region boundary  10 at:  -1.975E+00  1.132E+05
 ** GAS
    AQUEOUS
 ** HEMATITE

Phase region boundary  11 at:  -1.975E+00  1.132E+05
 ** GAS
    AQUEOUS
Calculated..                      9 equilibria
Terminating at axis limit.

Phase region boundary  12 at:  -1.975E+00  1.132E+05
    AQUEOUS
 ** HEMATITE
Calculated.                     30 equilibria

Phase region boundary  13 at:  -1.420E+01 -2.225E+04
    AQUEOUS
 ** HEMATITE
 ** MAGNETITE

Phase region boundary  14 at:  -1.420E+01 -2.225E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated..                     30 equilibria
Terminating at axis limit.

Phase region boundary  15 at:  -1.420E+01 -2.225E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                      4 equilibria

Phase region boundary  16 at:  -1.625E+01 -4.067E+04
 ** GAS
    AQUEOUS
 ** MAGNETITE

Phase region boundary  17 at:  -1.625E+01 -4.067E+04
    GAS
    AQUEOUS
 ** MAGNETITE
Calculated                     34 equilibria

Phase region boundary  18 at:  -1.625E+01 -4.067E+04
 ** GAS
    AQUEOUS
Calculated..                     28 equilibria
Terminating at axis limit.

Phase region boundary  19 at:  -1.625E+01 -4.067E+04
 ** GAS
    AQUEOUS
    MAGNETITE
Calculated..                     27 equilibria
Terminating at axis limit.

Phase region boundary  20 at:  -1.420E+01 -2.225E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
Calculated..                     30 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  21 at:  -1.975E+00  1.132E+05
    GAS
    AQUEOUS
 ** HEMATITE
Calculated                     11 equilibria

Phase region boundary  22 at:  -1.612E+01  7.817E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     19 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:  -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
```

```
Calculated..                      26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:  -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
Calculated.                        4 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:  -1.116E+01  1.000E+02
    AQUEOUS
 ** HEMATITE
Calculated.                        7 equilibria
Terminating at known equilibrium

Phase region boundary  26 at:  -1.116E+01  1.000E+02
    AQUEOUS
 ** HEMATITE
Calculated.                       24 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:  -1.612E+01 -2.701E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated..                      26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:  -1.612E+01 -2.701E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated.                        4 equilibria
Terminating at known equilibrium

Phase region boundary  29 at:  -1.612E+01 -3.959E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                        2 equilibria
Terminating at known equilibrium

Phase region boundary  30 at:  -1.612E+01 -3.959E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                        4 equilibria
Terminating at known equilibrium

Phase region boundary  31 at:  -1.485E+01 -2.840E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                        3 equilibria
Terminating at known equilibrium

Phase region boundary  32 at:  -1.485E+01 -2.840E+04
    AQUEOUS
 ** MAGNETITE
Calculated.                        2 equilibria
Terminating at known equilibrium

Phase region boundary  33 at:  -1.668E+01 -2.840E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated..                      26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  34 at:  -1.668E+01 -2.840E+04
    AQUEOUS
 ** HEMATITE
    MAGNETITE
Calculated.                        5 equilibria
Terminating at known equilibrium

Phase region boundary  35 at:  -9.172E+00  9.539E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                      35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  36 at:  -9.172E+00  9.539E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                       11 equilibria
Terminating at known equilibrium

Phase region boundary  37 at:  -9.210E+00  9.529E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                      35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  38 at:  -9.210E+00  9.529E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                       11 equilibria
Terminating at known equilibrium

Phase region boundary  39 at:  -9.210E+00  1.461E+04
    AQUEOUS
 ** HEMATITE
Calculated.                        8 equilibria
Terminating at known equilibrium

Phase region boundary  40 at:  -9.210E+00  1.461E+04
    AQUEOUS
 ** HEMATITE
```

```
Calculated.                     25 equilibria
Terminating at known equilibrium

Phase region boundary  41 at:  -9.210E+00 -2.323E+04
 ** GAS
    AQUEOUS
Calculated.                     10 equilibria
Terminating at known equilibrium

Phase region boundary  42 at:  -9.210E+00 -2.323E+04
 ** GAS
    AQUEOUS
Calculated..                     18 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  43 at:  -5.086E+00 -1.300E+04
 ** GAS
    AQUEOUS
Calculated.                     16 equilibria
Terminating at known equilibrium

Phase region boundary  44 at:  -5.086E+00 -1.300E+04
 ** GAS
    AQUEOUS
Calculated..                     13 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  45 at:  -1.293E+01 -1.300E+04
    AQUEOUS
 ** HEMATITE
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary  46 at:  -1.293E+01 -1.300E+04
    AQUEOUS
 ** HEMATITE
Calculated.                     27 equilibria
Terminating at known equilibrium

Phase region boundary  47 at:  -9.210E+00  9.623E+04
    GAS
    AQUEOUS
 ** HALITE
    HEMATITE
Calculated..                     33 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  48 at:  -9.210E+00  9.623E+04
    GAS
    AQUEOUS
 ** HALITE
    HEMATITE
Calculated.                     10 equilibria
Terminating at known equilibrium

Phase region boundary  49 at:  -9.210E+00  9.529E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  50 at:  -9.210E+00  9.529E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     11 equilibria
Terminating at known equilibrium

Phase region boundary  51 at:  -9.210E+00 -2.323E+04
 ** GAS
    AQUEOUS
Calculated.                     10 equilibria
Terminating at known equilibrium

Phase region boundary  52 at:  -9.210E+00 -2.323E+04
 ** GAS
    AQUEOUS
Calculated..                     18 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  53 at:  -9.210E+00  1.461E+04
    AQUEOUS
 ** HEMATITE
Calculated.                      8 equilibria
Terminating at known equilibrium

Phase region boundary  54 at:  -9.210E+00  1.461E+04
    AQUEOUS
 ** HEMATITE
Calculated.                     23 equilibria
Terminating at known equilibrium

Phase region boundary  55 at:  -1.975E+00  8.684E+04
    AQUEOUS
 ** HEMATITE
Calculated.                     26 equilibria
Terminating at known equilibrium

Phase region boundary  56 at:  -1.975E+00  8.684E+04
    AQUEOUS
 ** HEMATITE
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary  57 at:  -1.262E+01  8.684E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                     31 equilibria
Terminating at known equilibrium
```

```
Terminating at axis limit.

Phase region boundary  58 at:  -1.262E+01  8.684E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                      15 equilibria
Terminating at known equilibrium

Phase region boundary  59 at:  -1.612E+01  7.817E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                      26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  60 at:  -1.612E+01  7.817E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                      19 equilibria
Terminating at known equilibrium

Phase region boundary  61 at:  -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
Calculated..                      26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  62 at:  -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
 ** MAGNETITE
Calculated.                       4 equilibria
Terminating at known equilibrium

Phase region boundary  63 at:  -2.438E+00  6.600E+04
    AQUEOUS
 ** HEMATITE
Calculated.                      24 equilibria
Terminating at known equilibrium

Phase region boundary  64 at:  -2.438E+00  6.600E+04
    AQUEOUS
 ** HEMATITE
Calculated.                       9 equilibria
Terminating at known equilibrium

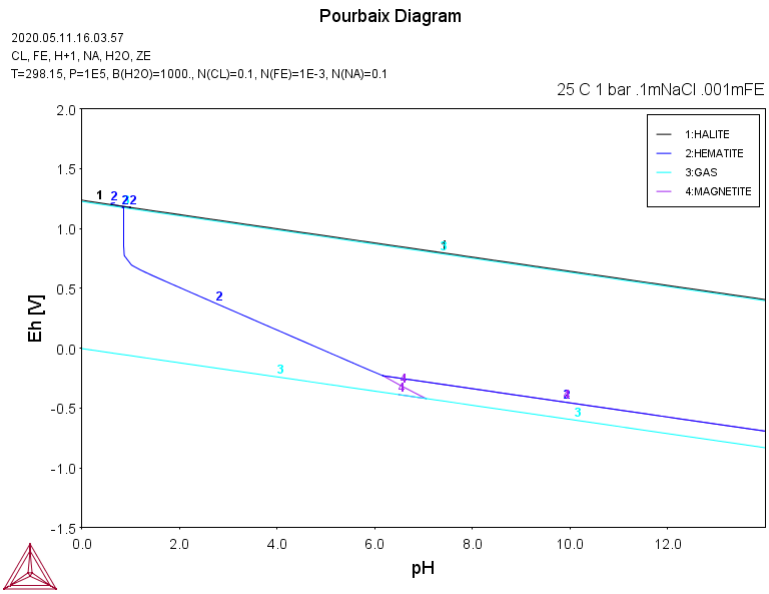
Phase region boundary  65 at:  -2.103E+01  6.600E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated..                      20 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  66 at:  -2.103E+01  6.600E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                      26 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex40\POURBAIX.POLY3
CPU time for mapping                   149 seconds
 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

CURRENT DEVICE: TC-UNITE Driver

Plotting the diagram; please be patient!
```



Hit RETURN to continue

Any missing phase boundary you could possibly think of? /N/: ?

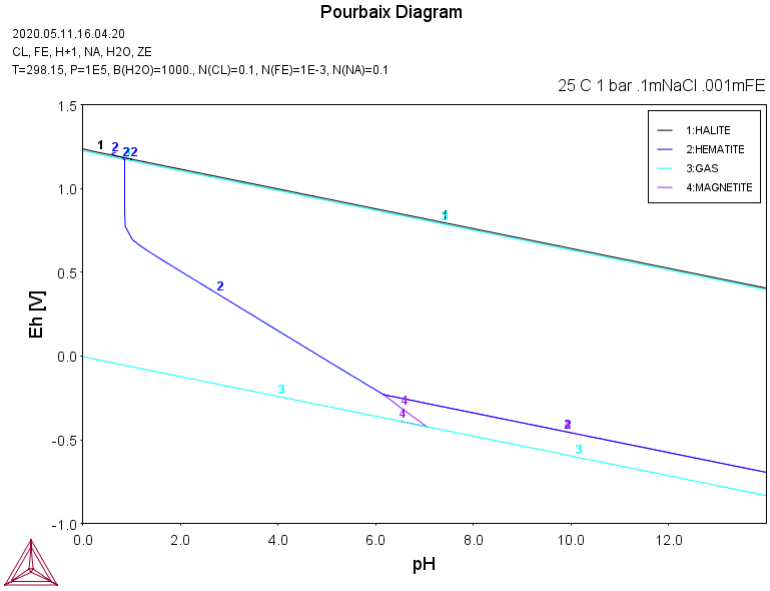
```
 ------------------------------------------------------------
 Sometimes the POURBAIX Module may miss some phase boundaries
   due to various reasons during the mapping process.
 By answering "Yes" here, the user would be able to add some
```

```
   additional starting point(s) into the calculation. In the
   following steps, the user will be asked to specify a pH-Eh
   coordinate pair, for instance (4.0, -0.15), which is close
   to the expected phase boundary.
 However, such additional pH-Eh point should not outside the
   AQUEOUS/GAS(O2) or AQUEOUS/GAS(H2) boundaries; otherwise,
   the module will fail in finding any new starting point.

Any missing phase boundary you could possibly think of? /N/: N

Change the pH/Eh steps for smoother curves? /N/: N

Zoom in? /N/: y
 Change scaling of X-axis? /N/: N
 Change scaling of Y-axis? /N/: y
  Minimum /-1.2/: -1.0
  Maximum /1.5/: 1.5
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
 CURRENT DEVICE: TC-UNITE Driver
 Plotting the diagram; please be patient!
```




```
Hit RETURN to continue

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: n

Save X-Y coordinates of curve on text file? /N/: y
File name /POURBAIX/: TCEX40-1.EXP
FILE EXISTS, OVERWRITE (Y OR N) /N/: Y

Modify the diagram? /N/: y

Zoom in? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: y

 At what pH-Eh point add the label text?
      X-pH /1.2/: 1.2
      Y-Eh /.25/: 0.25
  Automatic phase labels? /N/: N
      Text? /Aqs/: Aqs
Text size: /.36/: 0.26

Another Label Text to be added? /N/: y

 At what pH-Eh point add the label text?
      X-pH /2.599732093/: 8
      Y-Eh /.5/: 0.25
  Automatic phase labels? /N/: N
      Text? /Aqs/: Aqs+Hm
Text size: /.36/: 0.26

Another Label Text to be added? /N/: y

 At what pH-Eh point add the label text?
      X-pH /9.399732093/: 8
      Y-Eh /.5/: -0.3
  Automatic phase labels? /N/: N
      Text? /Aqs/: Aqs+Mt
Text size: /.36/: 0.26

Another Label Text to be added? /N/: y

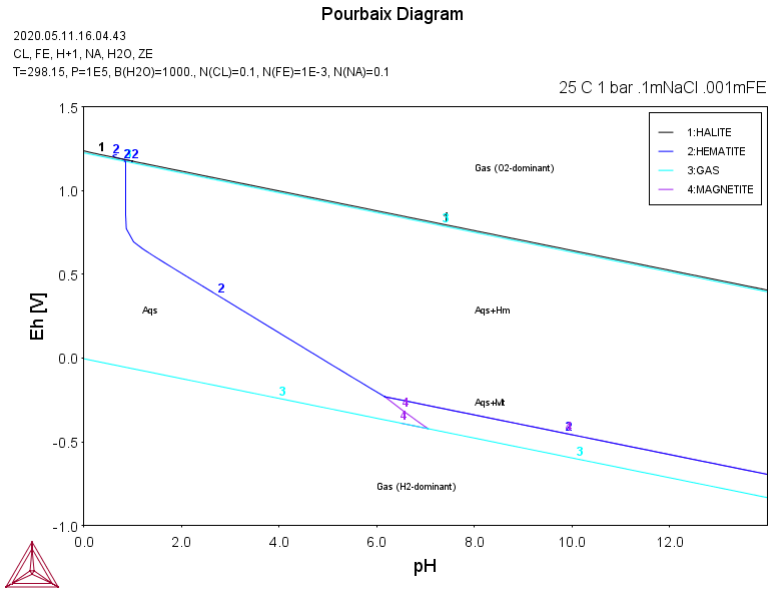
 At what pH-Eh point add the label text?
      X-pH /9.399732093/: 8
      Y-Eh /-.05/: 1.1
  Automatic phase labels? /N/: N
```

```
      Text? /Aqs/: Gas (O2-dominant)
Text size: /.36/: 0.26

Another Label Text to be added? /N/: y

 At what pH-Eh point add the label text?
      X-pH /9.399732093/: 6
      Y-Eh /1.35/: -.8
  Automatic phase labels? /N/: N
      Text? /Aqs/: Gas (H2-dominant)
Text size: /.36/: .26

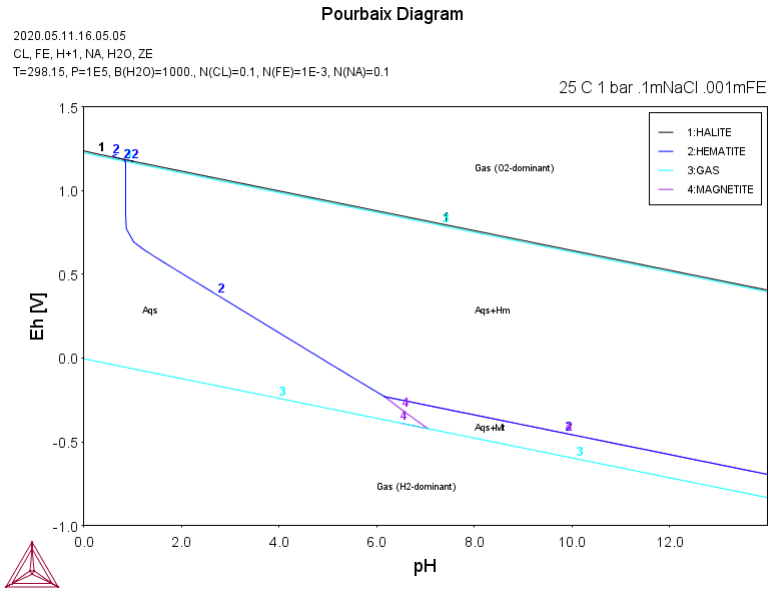
Another Label Text to be added? /N/: N
```




```
Hit RETURN to continue

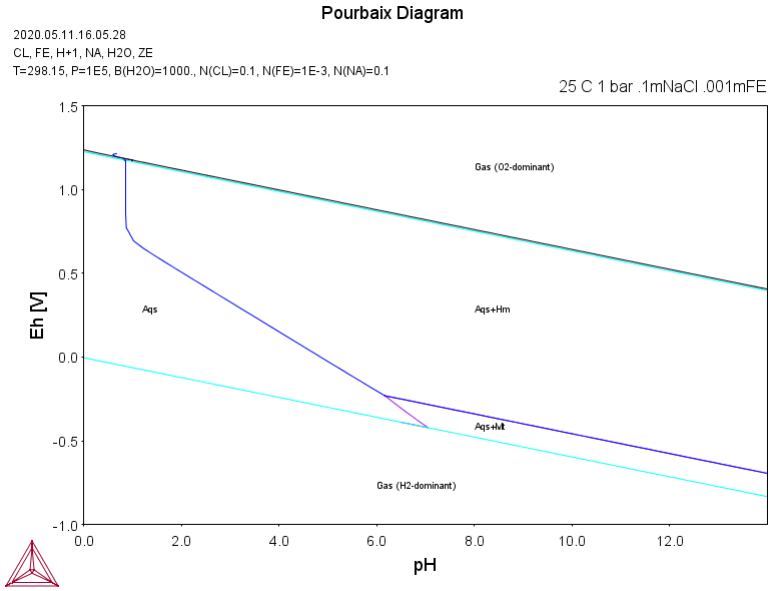
Modify Label-Texts on the Pourbaix diagram? /N/: y
 These labels are defined
 No   1 at  1.20000E+00 2.50000E-01 : Aqs
 No   2 at  8.00000E+00 2.50000E-01 : Aqs+Hm
 No   3 at  8.00000E+00-3.00000E-01 : Aqs+Mt
 No   4 at  8.00000E+00 1.10000E+00 : Gas (O2-dominant)
 No   5 at  6.00000E+00-8.00000E-01 : Gas (H2-dominant)
Which label to modify? /5/: 3
New X coordinate /8/: 8
New Y coordinate /-.3/: -.45
New text /Aqs+Mt/: Aqs+Mt

Another Label Text to be modified? /N/: N
```




```
Hit RETURN to continue

Modify Label-Curve-Option on the Pourbaix diagram? /N/: y
Curve-Label Option? /E/: ?
 THE OPTIONS MEANS:
 A     LIST STABLE PHASES ALONG LINE
 B     AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER
 C     LIST AXIS QUANTITIES
 D     AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER
 E     AS B WITH CHANGING COLORS
 F     AS D WITH CHANGING COLORS
 N     NO LABELS
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /E/: n
```




```
Hit RETURN to continue

Another Curve-Label Option? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: N

Modify Label-Texts on the Pourbaix diagram? /N/: N

Modify Label-Curve-Option on the Pourbaix diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: y

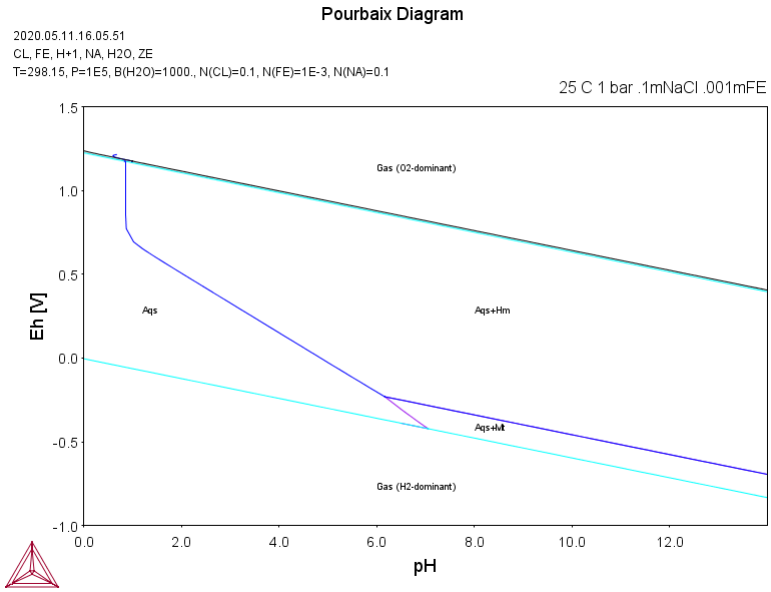
Zoom in? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: N

Modify Label-Texts on the Pourbaix diagram? /N/: y
 These labels are defined
 No   1 at  1.20000E+00 2.50000E-01 : Aqs
 No   2 at  8.00000E+00 2.50000E-01 : Aqs+Hm
 No   3 at  8.00000E+00-4.50000E-01 : Aqs+Mt
 No   4 at  8.00000E+00 1.10000E+00 : Gas (O2-dominant)
 No   5 at  6.00000E+00-8.00000E-01 : Gas (H2-dominant)
Which label to modify? /5/: 4
New X coordinate /8/: 6
New Y coordinate /1.1/: 1.1
New text /Gas (O2-dominant)/: Gas (O2-dominant)

Another Label Text to be modified? /N/: N
```




```
Hit RETURN to continue

Modify Label-Curve-Option on the Pourbaix diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N
```

```
Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: y

  Loading workspaces from the POLY3 file: POURBAIX

 The loaded POLY3 file is of POURBAIX-MAPPING Calculation.

 The current system consists of  6 elements:
    CL FE H  NA O  ZE

 List of Default and Pre-defined Calculation Conditions:
 ---------------------------------------------------------------
  Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole
 ---------------------------------------------------------------
 T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.1181, MUR(ZE)=66000.
 FIXED PHASES
 GAS=0
 DEGREES OF FREEDOM -1

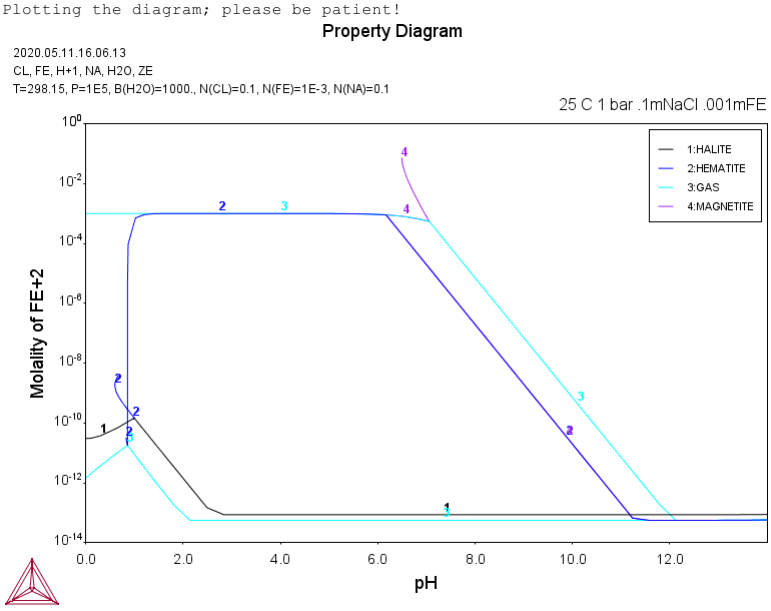
SET PLOTTING PARAMETERS:

   ------------------------------------------------------------
   I                                                          I
   I   The following properties are available to be selected  I
   I     as axis variables for making other diagrams from the I
   I     same calculation:                                    I
   I                                                          I
   I          pH  --- Acidity                                 I
   I          Eh  --- Electronic Potential [V]                I
   I          Ah  --- Electronic Affinity  [kJ]               I
   I          pe  --- Electronic Activity [log10ACRe]         I
   I          IS  --- Ionic Strength                          I
   I          TM  --- Total Concentration                     I
   I          Aw  --- Activity of Water                       I
   I          Oc  --- Osmotic Coefficient                     I
   I     MF(AQsp) --- Mole Fractions of aqueous species       I
   I     ML(AQsp) --- Molalities of aqueous species           I
   I     AI(AQsp) --- Activities of aqueous species           I
   I     RC(AQsp) --- Activity Coefficients of Aq Species     I
   I                                                          I
   I  where "AQsp" is the name of a specific aqueous species, I
   I    and "*" can be used as a wild sign for all "AQsp";    I
   I  It is unnecessary to give a complete aqueous species    I
   I    names; however, the entered AQsp name must be unique. I
   I  If neither "AQsp" nor "*" is given here, all species    I
   I    will be searched.                                     I
   I                                                          I
   I__________________________________________________________I

   List of all the AQsp (aqueous species) in the defined system:
   ==============================================================
    CL-1          CL2           CLO-1         CLO2          CLO2-1
    CLO3-1        CLO4-1        FE+2          FE+3          FE2O2H2+4
    FECL+2        FEO3H3-1      FEOH+1        FEOH+2        H+1
    H2            H2O           H2O2          HCLO          HCLO2
    HO2-1         NA+1          O2            O3            OH-1

   --------------------------------------------------------------

 X-axis Variable: /PH/: pH
 Y-axis Variable: /EH/: ml(fe+2)
 CURRENT DEVICE: TC-UNITE Driver
 Plotting the diagram; please be patient!
```

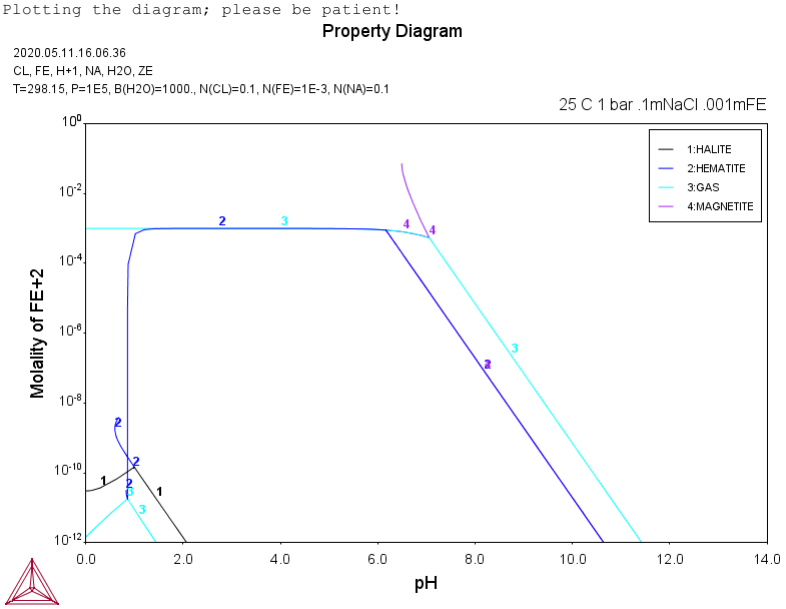



```
Hit RETURN to continue

Change axis type? /N/: N

Zoom in? /N/: y
 Change scaling of X-axis? /N/: y
  Minimum /0/: 0
  Maximum /13.99557858/: 14
 Change scaling of Y-axis? /N/: y
```

```
 Minimum /1E-40/: 1e-12
 Maximum /1/: 1e-2
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!
```




```
Hit RETURN to continue

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add label texts onto the specified diagram? /N/: N

Change the subtitle of the diagram? /N/: N

Change axis text? /N/: N

Further refine the diagram in POST module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: y


  Loading workspaces from the POLY3 file: POURBAIX

 The loaded POLY3 file is of POURBAIX-MAPPING Calculation.

 The current system consists of  6 elements:
    CL FE H  NA O  ZE

 List of Default and Pre-defined Calculation Conditions:
 ------------------------------------------------------------
  Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole
 ------------------------------------------------------------
 T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
    LNACR(H+1)=-16.1181, MUR(ZE)=66000.
 FIXED PHASES
 GAS=0
 DEGREES OF FREEDOM -1

SET PLOTTING PARAMETERS:

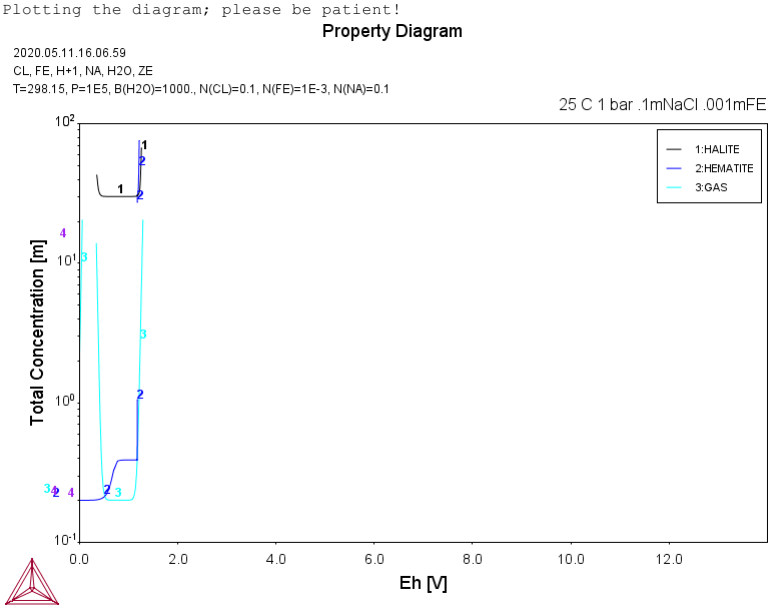
   ------------------------------------------------------------
   I                                                          I
   I   The following properties are available to be selected  I
   I     as axis variables for making other diagrams from the I
   I     same calculation:                                    I
   I                                                          I
   I          pH  --- Acidity                                 I
   I          Eh  --- Electronic Potential [V]                I
   I          Ah  --- Electronic Affinity  [kJ]               I
   I          pe  --- Electronic Activity [log10ACRe]         I
   I          IS  --- Ionic Strength                          I
   I          TM  --- Total Concentration                     I
   I          Aw  --- Activity of Water                       I
   I          Oc  --- Osmotic Coefficient                     I
   I     MF(AQsp) --- Mole Fractions of aqueous species       I
   I     ML(AQsp) --- Molalities of aqueous species           I
   I     AI(AQsp) --- Activities of aqueous species           I
   I     RC(AQsp) --- Activity Coefficients of Aq Species     I
   I                                                          I
   I  where "AQsp" is the name of a specific aqueous species, I
   I    and "*" can be used as a wild sign for all "AQsp";    I
   I  It is unnecessary to give a complete aqueous species    I
   I    names; however, the entered AQsp name must be unique. I
   I  If neither "AQsp" nor "*" is given here, all species    I
   I    will be searched.                                     I
   I                                                          I
   I__________________________________________________________I


   List of all the AQsp (aqueous species) in the defined system:
   ==============================================================
    CL-1          CL2           CLO-1         CLO2          CLO2-1
    CLO3-1        CLO4-1        FE+2          FE+3          FE2O2H2+4
    FECL+2        FEO3H3-1      FEOH+1        FEOH+2        H+1
```

```
H2          H2O         H2O2        HCLO        HCLO2
HO2-1       NA+1        O2          O3          OH-1

-----------------------------------------------------------------
```

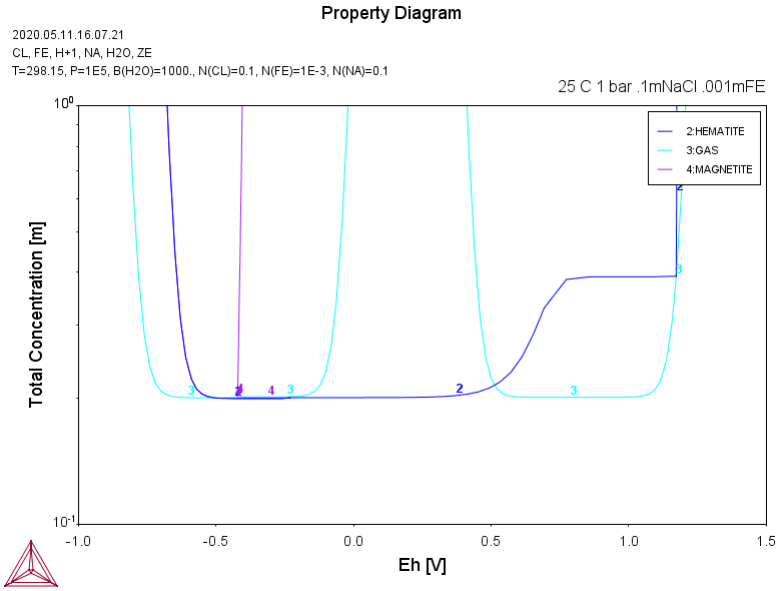
X-axis Variable: /PH/: Eh
Y-axis Variable: /ML/: TM
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!



Hit RETURN to continue

Change axis type? /N/: N

Zoom in? /N/: y
Change scaling of X-axis? /N/: y
Minimum /-1.2/: -1.0
Maximum /1.5/: 1.5
Change scaling of Y-axis? /N/: y
Minimum /1E-08/: 0.1
Maximum /100/: 1
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
CURRENT DEVICE: TC-UNITE Driver
Plotting the diagram; please be patient!



Hit RETURN to continue

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add label texts onto the specified diagram? /N/: N

Change the subtitle of the diagram? /N/: N

Change axis text? /N/: N

Further refine the diagram in POST module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: N

SYS:
SYS: @@... Up to this point, the POURBAIX module run is complete.

```
SYS:
SYS: SET_INTERACTIVE
   ... the command in full is SET_INTERACTIVE_MODE
SYS:
```

tcex41

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex41\tcex41.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculation of a solubility product
SYS:
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex41,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: def-mat
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: tcfe9
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: c .19
2nd alloying element: mn 1.16
Next alloying element: si .2
Next alloying element: cr .72
Next alloying element: ni .2
Next alloying element: mo .08
Next alloying element: cu .26
Next alloying element: al .027
Next alloying element: n .0089
Next alloying element:
Temperature (C) /1000/: 1056
 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
 REINITIATING GES .....
   ... 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                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M6C                     M5C2                    M3C2
 MC_ETA                  MC_SHP                  KSI_CARBIDE
 Z_PHASE                 FE4N_LP1                FECN_CHI
 PI                      SIGMA                   HIGH_SIGMA
 MU_PHASE                P_PHASE                 R_PHASE
 CHI_A12                 LAVES_PHASE_C14         M3SI
 MN9SI2                  MN11SI19                MN6SI
 G_PHASE                 CR3SI                   FE2SI
 FESI2_H                 FESI2_L                 MSI
 M5SI3                   NBNI3                   NI3TI
 AL2Y_C15                CU6Y                    MOSI2_C11B
 MO5SI3_D8M              AL8MN5_D810             NB5SI3_D8L
 MSI2_C40                M11SI8                  M6SI5
 KAPPA_E21               AL4C3                   FE8SI2C
 SIC                     MN5SIC                  CRZN17
 ZETA_FEZN               CUZN_EPSILON            BETA1
 GAMMA                   AL2FE1                  AL5FE4
 AL5FE2                  AL13FE4                 AL7CR
 AL2CR3                  ALN                     SI3N4
 MN6N4                   MN6N5                   MP_B31
 M2P_C22                 MULLITE:I               FLUORITE_C1:I
 ZRO2_TETR:I             M2O3C:I                 M2O3H:I
 CENI2                   CENI5
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                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE                M23C6                    M7C3
 M6C                      M5C2                     M3C2
 MC_ETA                   MC_SHP                   KSI_CARBIDE
 Z_PHASE                  FE4N_LP1                 FECN_CHI
 PI                       SIGMA                    HIGH_SIGMA
 MU_PHASE                 P_PHASE                  R_PHASE
 CHI_A12                  LAVES_PHASE_C14          M3SI
 MN9SI2                   MN11SI19                 MN6SI
 G_PHASE                  CR3SI                    FE2SI
 FESI2_H                  FESI2_L                  MSI
 M5SI3                    NBNI3                    NI3TI
 AL2Y_C15                 CU6Y                     MOSI2_C11B
 MO5SI3_D8M               AL8MN5_D810              NB5SI3_D8L
 MSI2_C40                 M11SI8                   M6SI5
 KAPPA_E21                AL4C3                    FE8SI2C
 SIC                      MN5SIC                   CRZN17
 ZETA_FEZN                CUZN_EPSILON             BETA1
 GAMMA                    AL2FE1                   AL5FE4
 AL5FE2                   AL13FE4                  AL7CR
 AL2CR3                   ALN                      SI3N4
 MN6N4                    MN6N5                    MP_B31
 M2P_C22                  MULLITE:I                FLUORITE_C1:I
 ZRO2_TETR:I              M2O3C:I                  M2O3H:I
 CENI2                    CENI5

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

OK? /Y/: Y
16:09:02,471 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set FCC_A1#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
 Creating a new composition set HCP_A3#2
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C as it has net charge
Suspending M2O3H as it has net charge
Suspending MULLITE as it has net charge
Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'M.H.G. Jacobs, P.J. Spencer, CALPHAD, 20 (1996) 307-320; Si-Zn and Al-Si
      -Zn'
  'N. Saunders, COST 507 Report (1998); Al-Cu'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE9
      database (TCFE v9.0, Jan, 2017).'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'J-O. Andersson, CALPHAD, 12 (1988) 1-8; TRITA 0317 (1986); C-MO'
  'Unassessed parameter; Linear combination of unary data'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'A. Fernandez Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362
      (1988); C-CO-NI AND C-CO-FE-NI'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
  'I. Ansara, Unpublished work (1991); Cr-Si'
  'J. Grobner, H.-L. Lukas, F. Aldinger, J. Alloys Compd., 220, 8-14 (1995);
      Y-Al-C'
  'D. Connetable, J. Lacaze, P. Maugis and B. Sundman; CALPHAD, 32 (2008)
      361-370; Al-C-Fe'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
  'Thermo-Calc Software, Sweden, 2019: Volume data updated for TCFE9
      database (TCFE v9.1, June, 2019).'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
  'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6
      database (TCFE v6, April, 2008).'
  'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C
      and Al-Si-C'
  'N. Subasic, Licentiate Thesis, KTH, Sweden, (2000)'
  'COST2 database 1997'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE8
      database (TCFE v8, May, 2015).'
  'M. Seiersten, Unpublished work (1989); Al-Fe'
  'I Ohnuma, unpublished work on B2 ordering (2001) Al-Fe'
  'B. Sundman, I. Ohnuma, N. Dupin, U.R. Kattner, S.G. Fries, Acta Mater. 57
      (2009) 2896-2908; Al-Fe'
  'B.B. Lindahl, M. Selleby, CALPHAD, 43, 86-93(2013); Al-Fe-Mn'
  'B. Sundman, Modified for wrong stoichiometry (2004) Al-Fe'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Al-Cr-Zn'
  'K.-G. Chin, H.-J. Lee, J.-H. Kwak, J.-Y. Kang, B.-J. Lee, J. Alloys
      Compd., 505, 217-23(2010); Al-Mn-C, Al-Fe-Mn-C'
  'Y. Du, J.C. Schuster, Z.K. Liu, R. Hu, P. Nash, W. Sun, et al.,
      Intermetallics. 16 (2008) 554-570.'
  'Y. Du, J. Wang, J. Zhao, J.C. Schuster, F. Weitzer, R. Schmid-Fetzer, M.
      Ohno, H. Xu, Z.-K. Liu, S. Shang, W. Zhang, Int. J. Mater. Res., 98,
```

855-71(2007); Al-Mn'
'A. Jansson, PhD Thesis, Stockholm 1997; Al-Fe-Mn'
'N. Saunders, COST 507 Report (1998); Al-Mo'
'M. Hillert and S. Jonsson, Metall. Trans. A, 23A (1992) 3141-3149; Al-Fe-N'
'Q. Chen and B. Sundman, J. Phase Equilib., 19 (2)(1998) 146-160'
'H.L. Lukas, COST 507 Report (1998); Al-N'
'B.-J. Lee, Private communication, (1999); Estimated parameter; Al-N'
'I. Ansara, N. Dupin, H.-L. Lukas and B. Sundman, J. Alloys Compd., 247 (1997) 20-30; Al-Ni'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
'N. Dupin, PhD Thesis, Institut National Polytechnique de Grenoble, (1995)'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the same phase as cubic Y2O3 (M2O3C).'
'H. Mao, M Selleby and B Sundman, J. Am. Cera. Soc., 88 (2005) 2544-2551; Al2O3-SiO2'
'TCS (2004), TCMP2 - TCS Materials Processing Database, v2, 2004.'
'S.H. Liu, Y. Du, H.L. Chen, CALPHAD, 30 (2006) 334-340; Al-Y'
'H. Mao, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
'C. Qiu, ISIJ International, 32 (1992) 1117-1127; C-Cr-Fe-Mo'
'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348, (1987); C-CR-FE-W'
'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.-J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
'P. Gustafson, Inst. Met. Res. (IM-2549, 1990); C-CU-FE'
'Chandrakasekan et. al, (1987) provisional; CU-FE-P-C'
'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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F. Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, submitted, 2011; Fe-Mn-C'
'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279 -85(2010); Mn-C'
'J.-H. Shim, C.-S. Oh, D.N. Lee, Metall. Mater. Trans. B. 27 (1996) 955 -966; Ti-Mo-C'
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci. (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218; TRITA-MAC 285 (1986); C-FE-NI'
'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53, 105-125; Molar volumes'
'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223; Fe-Si and Fe-Si-C'
'NPL, Unpublished work (1989); C-Mn-Si'
'W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Intermetallics. 15 (2007) 1401-1408.'
'H. Wang, Z. Li, Z. Chen, B. Yang, J. Phase Equilib. Diffus. 37 (2016) 1-7'
'K. Zeng and M. Hamalainen, CALPHAD, 19 (1995) 93-104; Cr-Cu'
'B. Sundman, Private communication, 2(1999); Estimated parameter'
'W.H. Sun, S.H. Liu, added to make this phase less stable, 2010'
'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270 (1986); CR-FE'
'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR -FE-N'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986); CR-FE-MO'
'B.-J. Lee, Private communication, (1999); Estimated parameter'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
'SGTE (2008): SSOL4 - SGTE Substance Database V4.1, provided by Thermo -Calc Software'
'K. Frisk, KTH Report D 60 (1984); CR-MO'
'B. Sundman, Private communication; FCC parameter same as BCC; Cr-Mo'
'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2015; LAVES_PHASE_C14'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Z_PHASE'
'K. Frisk, CALPHAD, 15 (1991) 79-106; TRITA-MAC 393 (1989); CR-N, FE-N, MO -N, CR-MO-N'
'Estimated parameter for solubility of N in cementite, 1999'
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
'I. Ansara and A. Jansson, TRITA-MAC 533 (1993); Cu-Fe'
'C.Y. He, J. Alloys Compd.,457,233-238 (2008); Cu-Mn'
'C.P. Wang, X.J. Liu, I. Ohnuma, R. Kainuma, K. Ishida, S.M. Hao, J. Phase Equilib. Diffus. 21 (2000) 54-62; Cu-Mo and Cu-Fe-Mo'
'Same or similar interaction as in the corresponding stable phase'
'K. Frisk, IM-2929, Swedish Inst. Met. Res., (1992); Cu-N, Fe-Cu-N'
'S. an Mey, CALPHAD, 16 (1992) 255-260; Cu-Ni'
'A. Jansson, TRITA-MAC 340 (1987); CU-FE-NI'
'M. Jacobs (1991), Revised by T. Buehler (1997), COST 507 Report; Cu-Si'
'S.G.Fries, H.L. Lukas, R. Konetzki, R. Schimd-Fetzer, J. Phase Equilib., 15 (1994) 606-614; Cu-Y'
'H. Mao, Thermo-Calc Software AB, Sweden, 2013; Molar volumes'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Unifying HCP_ZN with HCP_A3'
'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb and Fe-Mn-Nb'
'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
'A. Fernandez Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised 1986); TRITA-MAC 200 (1982); FE-MO'
'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
'H.K. Danielsen and J. Hald, CALPHAD, 31 (2007) 505-514; Z-PHASE'
'C. Qiu, Metall. Trans. A, 24A (1993) 629-645; Fe-Mn-N'
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'L. Zhang, Y. Du, H. Xu, S. Liu, Y. Liu, F. Zheng, et al., Int. J. Mater. Res. 100 (2009) 160-175; Fe-Mn-Ni'
'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe -Si-C'
'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'

```
  'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
  'C. Qiu and A. Fernandez Guillermet, Z. Metallkd., 84 (1993) 11-12; Mn-N'
  'A. Markstrom, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
  'S. Liu, Unpublished work (2010); Mn-Ni'
  'C.P. Guo,Intermetallics,13(5),525-534,(2005); Mn-Ni'
  'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
      -21; Mn-Y-O'
  'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
      -64; Mn-Zr-O, Mn-Y-Zr-O'
  'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
  'K. Frisk and B. Uhrenius, Metall. Mater. Trans. A, 27A (1996) 2869-2880;
      Mo-C-N, Fe-Mo-C-N'
  'K. Frisk, CALPHAD, 14 (1990) 311-320; MO-NI'
  'Y. Liu, G. Shao, P. Tsakiropoulos, Intermatallics 8 (2000) 953-962; Mo-Si,
       Al-Mo-Si'
  'A. Kusoffsky et al., Work within CCT-Applied Stainless steels, 2004; Fe
      -Cr-Si, Fe-Ni-Si, Fe-Cr-Cu, Fe-Cu-Mo, Cr-Mo-N-Ni, Fe-Cr-N-Ni, Fe-Al-Cr
      -Ni'
  'K. Frisk, Z. Metallkd., 82 (1991) 59-66; TRITA-MAC 414 (1989); Fe-Ni-N'
  'K. Frisk, Int. J. Thermophys., 12 (1990) 417-431; TRITA-MAC 419 (1990); N
      -NI'
  'X. Ma, C. Li, F. Wang, W. Zhang, CALPHAD, 27 (2003) 383-388; N-Si'
  'P. Gustafson, Inst. Met. Res. (Sweden) (1990); Estimations of C-CR-FE-V,
      C-CR-FE-MO-V-W, FE-N-W, FE-MN-N, FE-N-SI, CR-N-V, C-CR-N, FE-MO-N, CR
      -N-W, CR-TI-N'
  'Thermo-Calc Software, Sweden, 2009: Volume data updated for TCFE6
      database (TCFE v6, November, 2009).'
  'A. Bolcavage and U.R. Kattner, J. Phase Equilib., 2, (1996); Nb-Ni'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Estimated parameter;
       Ni-Zr-O'
  'P. Bellen, K.C. Hari Kumar and P. Wollants, Z. Metallkd., 87 (1994) 972
      -978; Ni-Ti'
  'J. Miettinen, CALPHAD, 27 (2003) 263-274; Cu-Ni-Zn'
  'H.Liang, Y.A.Chang, J. Phase Equilib. 19 (1998) 25-37'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; Fe-Al-Cr-Ni'
  'H-L Chen, J. Mater. Res., 24(10) 3154-3164 (2009); Al-Cu-Fe'
  'C.-Y. He, unpublished work (2008), Al-Cu-Mn'
  'H-L Chen, unpublished work (2007), Al-Cu-Ni'
  'N. Dupin 2008'
  'L. Kjellqvist and M. Selleby, Unpublished research (2013); Al-Fe-Si-O'
  'H-L Chen, Thermo-Calc Software AB, Sweden, 2013; Al-Mn-Ni'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-V-W-C'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; C-Cr-Si'
  'S. Nagakura, Transactions of the Iron and Steel Institute of Japan, 8
      (1968) 265-294; Molar volumes'
  'I.K. Kupalova, V.I. Pavlova, High Speed Steels: Physical Properties,
      Prop. Data Updat. 2 (1988) 67-78; Molar volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid
      C-Fe-Si description'
  'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
  'C.P. Wang, D.X. Huang, J.J. Zhu, S.Y. Yang, X.J. Liu, J. Phase Equilib.
      Diffus. 35 (2014) 314-325; Cr-Cu-Mo and Cr-Cu-W'
  'T. Ikoma, M. Kajihara, Mater. Sci. Eng. A. 437 (2006) 293-300; Cr-Cu-Ni'
  'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
  'A. Markstrom, Thermo-Calc Software AB, Sweden, 2013; Extrapolations,
      assumptions and adjustment'
  'B. Sundman, Private communication, (2000); Estimated Cr-Ni-Mo'
  'B.-J. Lee, Private communication, (2000); Estimated parameter'
  'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; Fe-Cr-N, Fe
      -C-Cr-N, Fe-Cr-Mo-N, Fe-Cr-Mn-N'
  'K. Frisk, TRITA-MAC 422 (1990); CR-FE-N-NI'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Fe-Cr-Ni'
  'J. Miettinen, CALPHAD, 23 (2)(1999) 249-262; Cr-Fe-Si'
  'L. Zhang, Y. Du, Q. Chen, H. Xu, F. Zheng, C. Tang, H. Chen, Int. J.
      Mater. Res. 99 (2008) 1306-1318; Cu-Fe-Mn'
  'J. Miettinen, CALPHAD, 27 (2003) 389-394, Cu-Fe-Si'
  'W.H. Sun, CALPHAD, 33 (2009) 642-649; Cu-Mn-Ni'
  'K. Frisk, TRITA-MAC 433 (1990); FE-CR-MO-NI-N'
  'J. Miettinen, CALPHAD, 22 (1998) 275-300; Fe-Mo-Si'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Fe-Nb-Si'
  'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
      Fe-P-Si'
  'B. Hu, Unpublished (2010); Mn-Ni-Si,Al-Cu-Fe-Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
      M23C6'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Solubilities in M6C'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         47362 grid points in             4 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       3 s, total time     7  s
POLY:

POLY: l-e,,,
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -6.89244E+04,  Enthalpy  3.91313E+04,  Volume  7.33526E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      5.5361E-04  2.7000E-04 1.6231E-09 -2.2366E+05 SER
 C                       8.7517E-03  1.9000E-03 8.6820E-03 -5.2455E+04 SER
 CR                      7.6609E-03  7.2000E-03 7.6587E-05 -1.0473E+05 SER
 CU                      2.2636E-03  2.6000E-03 1.0228E-04 -1.0154E+05 SER
 FE                      9.6245E-01  9.7154E-01 2.2977E-03 -6.7145E+04 SER
 MN                      1.1682E-02  1.1600E-02 1.1143E-05 -1.2604E+05 SER
 MO                      4.6133E-04  8.9000E-04 1.0052E-05 -1.2717E+05 SER
 N                       3.5153E-04  8.9000E-05 5.2295E-07 -1.5984E+05 SER
 NI                      1.8853E-03  2.0000E-03 2.8002E-06 -1.4130E+05 SER
 SI                      3.9396E-03  2.0000E-03 5.0704E-09 -2.1108E+05 SER

 FCC_A1#1                     Status ENTERED     Driving force  0.0000E+00
 Moles 9.9974E-01, Mass 5.5319E+01, Volume fraction 9.9978E-01  Mass fractions:
```

```
 FE  9.71633E-01  CR  7.20068E-03  SI  2.00019E-03  C   1.90018E-03  AL  2.07436E-04
 MN  1.16011E-02  CU  2.60025E-03  NI  2.00019E-03  MO  8.00076E-04  N   5.65165E-05

 ALN                        Status ENTERED     Driving force  0.0000E+00
 Moles 2.5665E-04, Mass 5.2599E-03, Volume fraction 2.2339E-04  Mass fractions:
 AL  6.58274E-01  SI  0.00000E+00  MO  0.00000E+00  FE  0.00000E+00  CR  0.00000E+00
 N   3.41726E-01  NI  0.00000E+00  MN  0.00000E+00  CU  0.00000E+00  C   0.00000E+00
POLY:Hit RETURN to continue
POLY:
POLY: def-dia
   ... the command in full is DEFINE_DIAGRAM
Same elements as before? /Y/: Y
 For binary or ternary diagrams you may prefer the special modules

 You must specify a value for all compositions and the temperature even
 if you want to use it as axis.
Mass (weight) percent of AL /.027/: .027
Mass (weight) percent of C /.19/: .19
Mass (weight) percent of CR /.72/: .72
Mass (weight) percent of CU /.26/: .26
Mass (weight) percent of MN /1.16/: 1.16
Mass (weight) percent of MO /.08/: .08
Mass (weight) percent of N /.0089/: .0089
Mass (weight) percent of NI /.2/: .2
Mass (weight) percent of SI /.2/: .2
Temperature (C) /1056/: 1056
 Using global minimization procedure
 Using already calculated grid
Found the set of lowest grid points in              0 s
 Calculated POLY solution       1 s, total time     1  s
 You must now set an independent axis for your diagram
 as one of the following conditions:
 Condition  1 is temperature (Celsius)
 Condition  2 is mass percent of C
 Condition  3 is mass percent of MN
 Condition  4 is mass percent of SI
 Condition  5 is mass percent of CR
 Condition  6 is mass percent of NI
 Condition  7 is mass percent of MO
 Condition  8 is mass percent of CU
 Condition  9 is mass percent of AL
 Condition 10 is mass percent of N
Give the number of the condition to vary /1/: 1
Minimum value (C) /800/: 650
Maximum value (C) /1800/: 1200

 The second axis can be another of the conditions above and you will then
 calculate a phase diagram.
 Or you may want to plot how some other quantities depend on the selected
 condition and you will then calculate a  "property" diagram.

 In addition to the conditions above you may use these selected
 dependent quantities on the vertical axis:
 Dependent 11 is mass fraction of all phases
 Dependent 12 is composition of a phase
 Dependent 13 is the fraction of a component in all phases
 (In the post processor you may select many other quantities)
Give the number of the quantity on second axis /11/: 11 tcex41
 No initial equilibrium, using default
 Step will start from axis value    1329.15
...OK

 Phase Region from    1329.15     for:
     ALN
     FCC_A1#1
 Global check of removing phase at  1.38366E+03
 Calculated     8 equilibria

 Phase Region from    1383.66     for:
     FCC_A1#1
 Global test at  1.45915E+03 .... OK
 Terminating at    1473.15
 Calculated    13 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  1.07178E+03
 Calculated    28 equilibria

 Phase Region from    1071.78     for:
     ALN
     BCC_A2
     FCC_A1#1
 Global test at  9.99150E+02 .... OK
 Global check of adding phase at  9.94423E+02
 Calculated    11 equilibria

 Phase Region from    994.423     for:
     ALN
     BCC_A2
     CEMENTITE
     FCC_A1#1
 Global check of removing phase at  9.67779E+02
 Calculated     6 equilibria

 Phase Region from    967.779     for:
     ALN
     BCC_A2
     CEMENTITE
 Terminating at    923.150
 Calculated     8 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex41\tcex41.POLY3
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

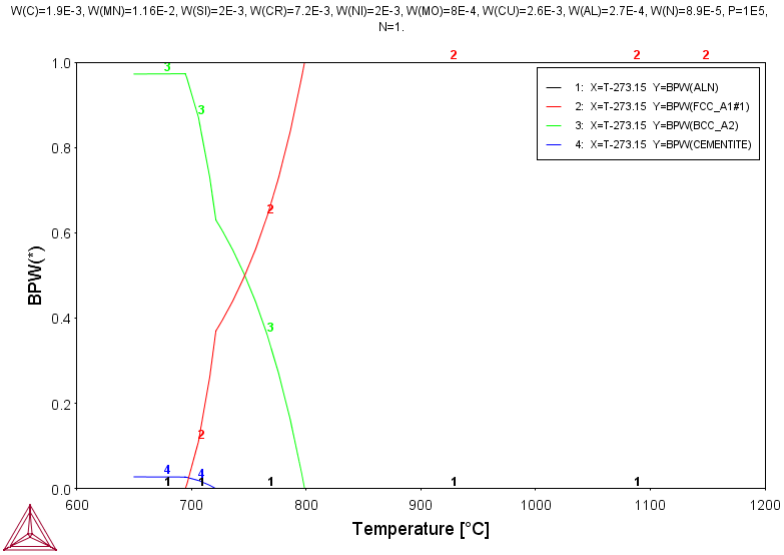
   ... the command in full is REINITIATE_PLOT_SETTINGS
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

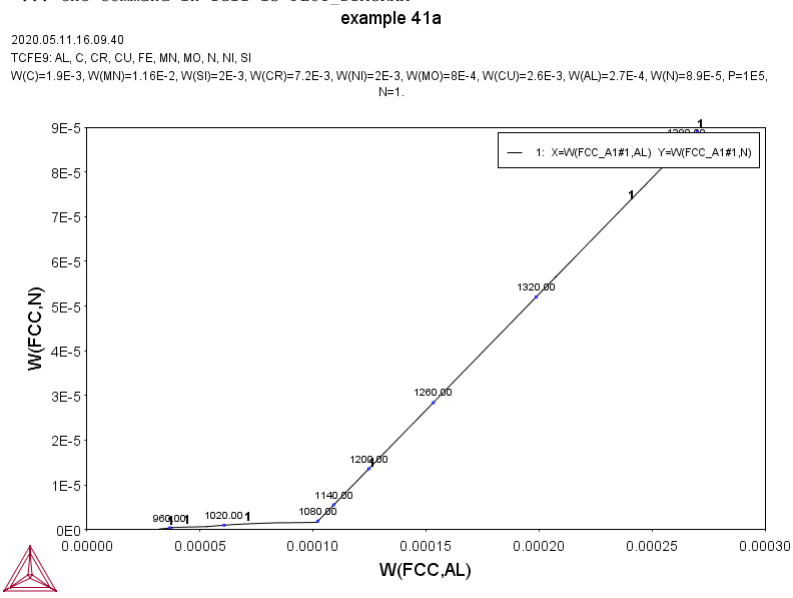
   ... the command in full is SET_AUTOMATIC_DIAGRAM_A
```

```
Setting automatic diagram axes

   ... the command in full is PLOT_DIAGRAM
```

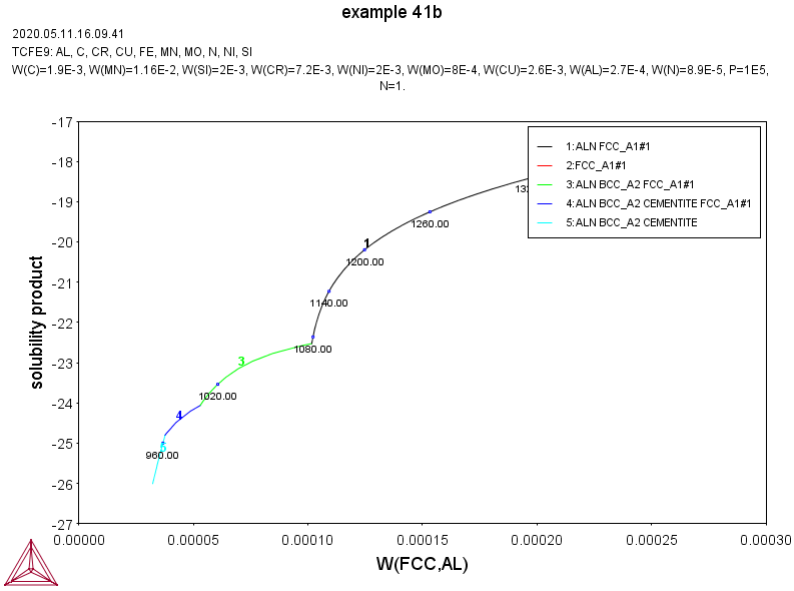



```
POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a x w(fcc,al)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(fcc,n)
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-d-a z t
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 1250 1350
   ... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 41a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Now let's go back to POLY3 and enter a function
POST: @@ corresponding to the solubillity product
POST: back
POLY: enter fun
   ... the command in full is ENTER_SYMBOL
Name: sp
Function: log(w(fcc,al)*w(fcc,n));
POLY:
POLY: @@ Now go back to POST and plot the entered function
POLY: post
POST:
POST: s-d-a y sp
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-t-s y n solubility product
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
```

```
POST: set-title example 41b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex42

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex42\tcex42.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Paraequilibrium calculation - Formation of Para-pearlite - Isopleth
SYS:
SYS: @@ This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to
SYS: @@ show a paraequilibrium calculation where there is formation of
SYS: @@ para-pearlite. It is an isopleth calculation and shows the
SYS: @@ Step_with_Options command using the Paraequilibrium option.
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex42,,,
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw tcfe9
   ... the command in full is SWITCH_DATABASE
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: d-sys fe c mn
   ... the command in full is DEFINE_SYSTEM
 FE                      C                       MN
   DEFINED
TDB_TCFE9: rej ph gra m5c2 diamond_fcc_a4
   ... the command in full is REJECT
 GRAPHITE                M5C2                    DIAMOND_FCC_A4
   REJECTED
TDB_TCFE9: get
   ... the command in full is GET_DATA
16:10:58,708 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 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
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C as it has net charge
Suspending M2O3H as it has net charge
Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE9
      database (TCFE v9.0, Jan, 2017).'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'M. Seiersten, Unpublished work (1989); Al-Fe'
  'Unassessed parameter; Linear combination of unary data'
  '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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-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'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
      and Fe-Mn-Nb'
  'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
      solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
      same phase as cubic Y2O3 (M2O3C).'
  'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
      -21; Mn-Y-O'
```

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  'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
      -64; Mn-Zr-O, Mn-Y-Zr-O'
  'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE8
      database (TCFE v8, May, 2015).'
 -OK-
TDB_TCFE9: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:

POLY: @@ To work with u-fractions, just set the status of component C to SPECIAL
POLY:
POLY: c-s com c
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: special
POLY: l-st
   ... the command in full is LIST_STATUS
Option /CPS/:
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)            P(Pa)
 VA                       ENTERED   SER
 C                        SPECIAL   SER
 FE                       ENTERED   SER
 MN                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 M7C3                     ENTERED      0.000000E+00    0.000000E+00
 M23C6                    ENTERED      0.000000E+00    0.000000E+00
 LAVES_PHASE_C14          ENTERED      0.000000E+00    0.000000E+00
 KSI_CARBIDE              ENTERED      0.000000E+00    0.000000E+00
 HCP_A3                   ENTERED      0.000000E+00    0.000000E+00
 G_PHASE                  ENTERED      0.000000E+00    0.000000E+00
 FECN_CHI                 ENTERED      0.000000E+00    0.000000E+00
 FE4N_LP1                 ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                   ENTERED      0.000000E+00    0.000000E+00
 CUZN_EPSILON             ENTERED      0.000000E+00    0.000000E+00
 CUB_A13                  ENTERED      0.000000E+00    0.000000E+00
 CEMENTITE                ENTERED      0.000000E+00    0.000000E+00
 CBCC_A12                 ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                   ENTERED      0.000000E+00    0.000000E+00
 AL5FE4                   ENTERED      0.000000E+00    0.000000E+00
 LIQUID                   ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 *** STATUS FOR ALL SPECIES
 C    ENTERED    C4   ENTERED    FE   ENTERED    FE+4 ENTERED    MN+3 ENTERED
 C2   ENTERED    C5   ENTERED    FE+2 ENTERED    MN   ENTERED    MN+4 ENTERED
 C3   ENTERED    C60  ENTERED    FE+3 ENTERED    MN+2 ENTERED    VA   ENTERED
POLY:
POLY:Hit RETURN to continue
POLY: s-c t=900 p=1e5 n=1 w(c)=0.002 w(mn)=0.025
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         17572 grid points in             2 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     2  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -3.64344E+04,  Enthalpy  2.02443E+04,  Volume  7.24781E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        9.2099E-03  2.0000E-03 1.6686E-01 -1.3399E+04 SER
 FE                       9.6562E-01  9.7500E-01 8.1714E-03 -3.5972E+04 SER
 MN                       2.5169E-02  2.5000E-02 2.3252E-04 -6.2607E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.6367E-01, Mass 5.3797E+01, Volume fraction 9.6992E-01  Mass fractions:
 FE  9.81934E-01  MN  1.80378E-02  C   2.86448E-05

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 3.6326E-02, Mass 1.6238E+00, Volume fraction 3.0085E-02  Mass fractions:
 FE  6.78866E-01  MN  2.53958E-01  C   6.71754E-02
POLY: s-a-v 1 w(c) 0 0.02
   ... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/: 2.5E-04
POLY: s-a-v 2 t 800 1200 10
   ... the command in full is SET_AXIS_VARIABLE
POLY: sa tcex42a y
   ... the command in full is SAVE_WORKSPACES
POLY: map
 Version S mapping is selected
 Generating start equilibrium  1
 Generating start equilibrium  2
 Generating start equilibrium  3
 Generating start equilibrium  4
 Generating start equilibrium  5
 Generating start equilibrium  6
 Generating start equilibrium  7
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
```
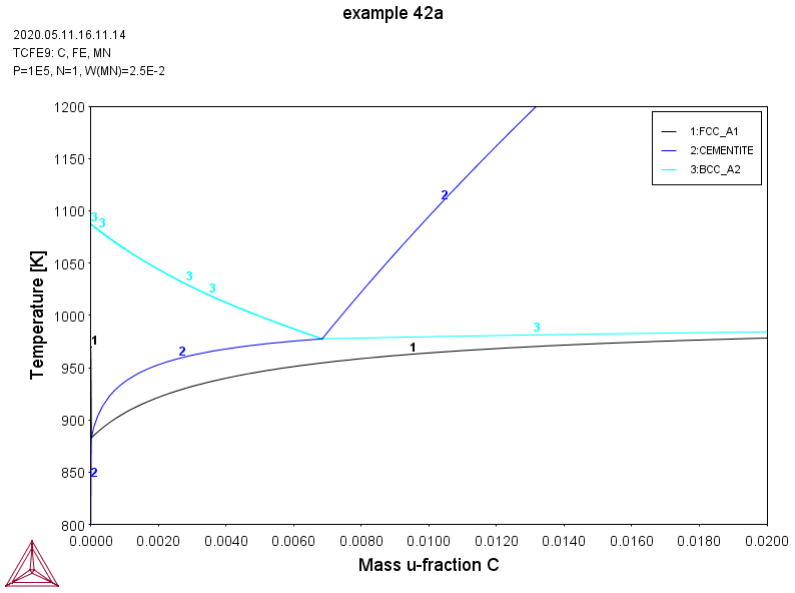

```
Generating start point   4
Generating start point   5
Generating start point   6
Generating start point   7
Generating start point   8
Generating start point   9
Generating start point  10
Working hard
Generating start point  11
Generating start point  12
Generating start point  13
Generating start point  14
Generating start point  15
Generating start point  16
Generating start point  17
Generating start point  18
Generating start point  19
Generating start point  20
Working hard
Generating start point  21
Generating start point  22
Generating start point  23
Generating start point  24
Generating start point  25
Generating start point  26
Generating start point  27
Generating start point  28
Generating start point  29
Generating start point  30
Working hard
Working hard

Phase region boundary   1 at:   2.500E-04  8.899E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                      3 equilibria

Phase region boundary   2 at:   1.688E-05  8.830E+02
    BCC_A2
 ** CEMENTITE
 ** FCC_A1

Phase region boundary   3 at:   1.688E-05  8.830E+02
    BCC_A2
 ** FCC_A1
Calculated                      24 equilibria

Phase region boundary   4 at:   1.688E-05  8.830E+02
    BCC_A2
 ** CEMENTITE
Calculated..                     10 equilibria
Terminating at axis limit.

Phase region boundary   5 at:   1.688E-05  8.830E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                      33 equilibria

Phase region boundary   6 at:   6.844E-03  9.776E+02
 ** BCC_A2
 ** CEMENTITE
    FCC_A1

Phase region boundary   7 at:   6.844E-03  9.776E+02
 ** CEMENTITE
    FCC_A1
Calculated..                     38 equilibria
Terminating at axis limit.

Phase region boundary   8 at:   6.844E-03  9.776E+02
 ** BCC_A2
    FCC_A1
Calculated                      46 equilibria

Phase region boundary   9 at:   6.844E-03  9.776E+02
 ** BCC_A2
    CEMENTITE
    FCC_A1
Calculated..                     54 equilibria
Terminating at axis limit.

Phase region boundary  10 at:   1.688E-05  8.830E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     85 equilibria
Terminating at axis limit.

Phase region boundary  11 at:   2.500E-04  8.899E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     81 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  12 at:   6.750E-03  9.543E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                      31 equilibria
Terminating at known equilibrium

Phase region boundary  13 at:   6.750E-03  9.543E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                     55 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  14 at:   1.325E-02  9.705E+02
    BCC_A2
    CEMENTITE
```

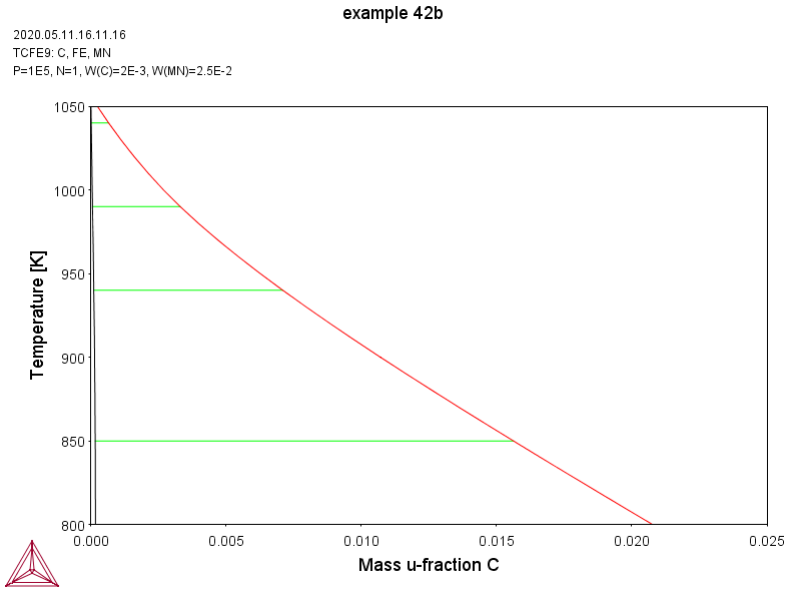
```
 ** FCC_A1
Calculated.                      54 equilibria
Terminating at known equilibrium

Phase region boundary  15 at:   1.325E-02  9.705E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                      29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  16 at:   3.169E-06  8.100E+02
    BCC_A2
 ** CEMENTITE
Calculated..                       3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  17 at:   3.169E-06  8.100E+02
    BCC_A2
 ** CEMENTITE
Calculated.                       9 equilibria
Terminating at known equilibrium

Phase region boundary  18 at:   1.975E-02  9.781E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                      83 equilibria
Terminating at known equilibrium

Phase region boundary  19 at:   1.975E-02  9.781E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                       3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  20 at:   1.009E-03  9.367E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                       8 equilibria
Terminating at known equilibrium

Phase region boundary  21 at:   1.009E-03  9.367E+02
    BCC_A2
 ** CEMENTITE
    FCC_A1
Calculated.                      28 equilibria
Terminating at known equilibrium

Phase region boundary  22 at:   3.541E-03  9.367E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated.                      16 equilibria
Terminating at known equilibrium

Phase region boundary  23 at:   3.541E-03  9.367E+02
    BCC_A2
    CEMENTITE
 ** FCC_A1
Calculated..                      68 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  24 at:   1.020E-03  1.063E+03
 ** BCC_A2
    FCC_A1
Calculated.                      32 equilibria
Terminating at known equilibrium

Phase region boundary  25 at:   1.020E-03  1.063E+03
 ** BCC_A2
    FCC_A1
Calculated                     21 equilibria

Phase region boundary  26 at:   9.115E-03  1.063E+03
 ** CEMENTITE
    FCC_A1
Calculated.                      11 equilibria
Terminating at known equilibrium

Phase region boundary  27 at:   9.115E-03  1.063E+03
 ** CEMENTITE
    FCC_A1
Calculated..                      29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  28 at:   1.287E-02  1.190E+03
 ** CEMENTITE
    FCC_A1
Calculated.                      36 equilibria
Terminating at known equilibrium

Phase region boundary  29 at:   1.287E-02  1.190E+03
 ** CEMENTITE
    FCC_A1
Calculated..                       4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary  30 at:   2.500E-04  1.081E+03
 ** BCC_A2
    FCC_A1
Calculated                       4 equilibria

Phase region boundary  31 at:   2.500E-04  1.081E+03
 ** BCC_A2
    FCC_A1
Calculated.                      28 equilibria
Terminating at known equilibrium
```

```
 Phase region boundary  32 at:   6.750E-03  9.786E+02
  ** BCC_A2
     FCC_A1
 Calculated                     30 equilibria

 Phase region boundary  33 at:   6.750E-03  9.786E+02
  ** BCC_A2
     FCC_A1
 Calculated.                     2 equilibria
 Terminating at known equilibrium

 Phase region boundary  34 at:   1.325E-02  9.814E+02
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated.                    27 equilibria
 Terminating at known equilibrium

 Phase region boundary  35 at:   1.325E-02  9.814E+02
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated..                    29 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  36 at:   1.287E-02  1.190E+03
  ** CEMENTITE
     FCC_A1
 Calculated.                    36 equilibria
 Terminating at known equilibrium

 Phase region boundary  37 at:   1.287E-02  1.190E+03
  ** CEMENTITE
     FCC_A1
 Calculated..                     4 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  38 at:   1.975E-02  9.841E+02
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated.                    53 equilibria
 Terminating at known equilibrium

 Phase region boundary  39 at:   1.975E-02  9.841E+02
  ** BCC_A2
     CEMENTITE
     FCC_A1
 Calculated..                     3 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex42\tcex42a.POLY3
 CPU time for mapping                    12 seconds
POLY: po
   ... the command in full is POST
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-lab e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-text x n Mass u-fraction C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-title example 42a
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

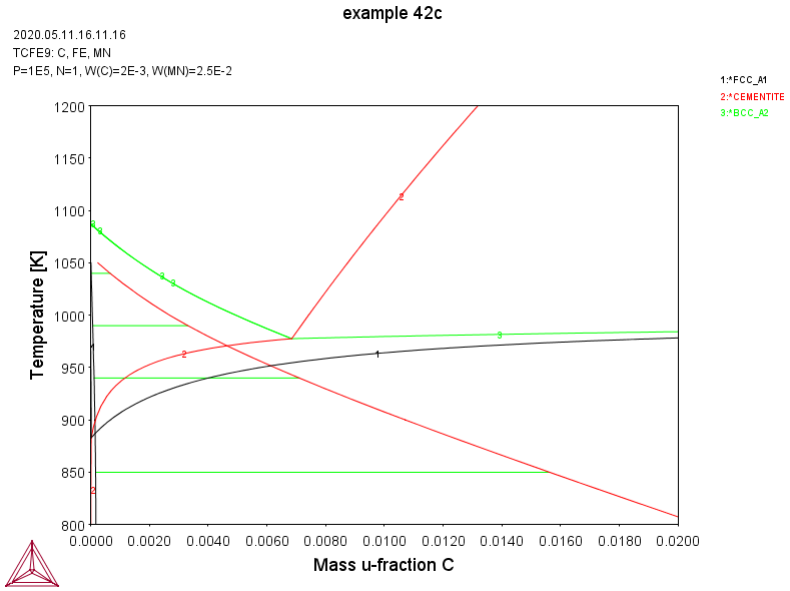



```
POST:
POST:Hit RETURN to continue
POST:
POST: make tcex42 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
```

```
POST: back
POLY: read tcex42a
   ... the command in full is READ_WORKSPACES
POLY: s-a-v 1 t 800 1200 10
   ... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY: sa tcex42b y
   ... the command in full is SAVE_WORKSPACES
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824   4.978869E-02   6.632643E-04  -2.411057E-01
   8.900000E+02    0.161    0.839   5.422687E-02   6.913508E-04  -2.813704E-02
   8.800000E+02    0.148    0.852   5.873901E-02   7.164951E-04   1.826502E-01
   8.700000E+02    0.137    0.863   6.331566E-02   7.386280E-04   3.918260E-01
   8.600000E+02    0.127    0.873   6.794838E-02   7.577054E-04   5.998954E-01
   8.500000E+02    0.119    0.881   7.262964E-02   7.737057E-04   8.073109E-01
   8.400000E+02    0.111    0.889   7.735275E-02   7.866282E-04   1.014482E+00
   8.300000E+02    0.105    0.895   8.211172E-02   7.964907E-04   1.221785E+00
   8.200000E+02    0.099    0.901   8.690123E-02   8.033288E-04   1.429564E+00
   8.100000E+02    0.093    0.907   9.172101E-02   8.071896E-04   1.638138E+00
   8.000000E+02    0.089    0.911   9.656384E-02   8.081409E-04   1.847814E+00

 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824   4.978869E-02   6.632643E-04  -2.411057E-01
   9.100000E+02    0.193    0.807   4.543503E-02   6.323326E-04  -4.569059E-01
   9.200000E+02    0.214    0.786   4.117770E-02   5.986843E-04  -6.762872E-01
   9.300000E+02    0.239    0.761   3.702982E-02   5.624832E-04  -9.001238E-01
   9.400000E+02    0.270    0.730   3.300598E-02   5.239339E-04  -1.129448E+00
   9.500000E+02    0.308    0.692   2.912230E-02   4.832877E-04  -1.365490E+00
   9.600000E+02    0.355    0.645   2.539648E-02   4.408500E-04  -1.609739E+00
   9.700000E+02    0.415    0.585   2.184787E-02   3.969899E-04  -1.864015E+00
   9.800000E+02    0.493    0.507   1.849747E-02   3.521517E-04  -2.130571E+00
   9.900000E+02    0.597    0.403   1.536779E-02   3.068684E-04  -2.412226E+00
   1.000000E+03    0.739    0.261   1.248280E-02   2.617798E-04  -2.712534E+00
   1.010000E+03    0.942    0.058   9.854684E-03   2.173469E-04  -3.037411E+00
   1.020000E+03    1.258   -0.258   7.421980E-03   1.722922E-04  -3.406145E+00
   1.030000E+03    1.821   -0.821   5.162055E-03   1.261990E-04  -3.851525E+00
   1.040000E+03    3.087   -2.087   3.064317E-03   7.893021E-05  -4.452554E+00
   1.050000E+03    8.516   -7.516   1.118313E-03   3.035996E-05  -5.537475E+00
 *** Buffer savend on file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex42\TCEX42~2.POL
 *** ERROR     3 IN NS01AD: Numerical error
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n Mass u-fraction C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 42b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

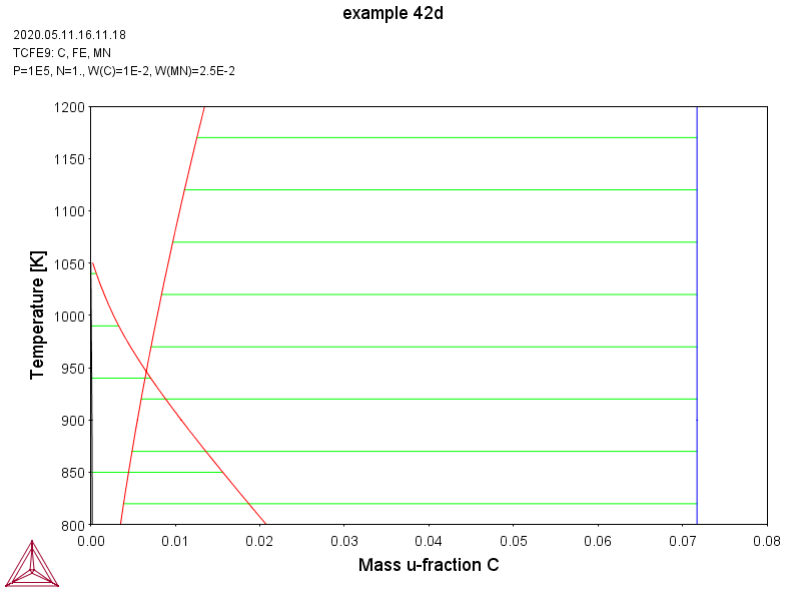



```
POST:
POST:Hit RETURN to continue
POST:
POST: ap-e y tcex42
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.02
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 800 1200
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 42c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

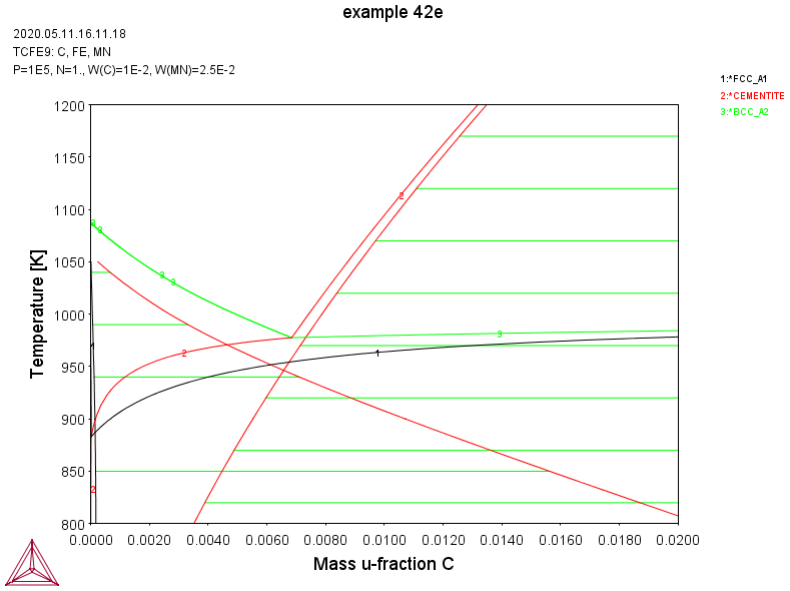



```
POST:Hit RETURN to continue
POST:
POST: back
POLY: read tcex42b
   ... the command in full is READ_WORKSPACES
POLY: s-c w(c)=0.01
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         17572 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -3.55310E+04,  Enthalpy  2.03102E+04,  Volume  7.05497E-06
```

```
 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        4.4413E-02  1.0000E-02 2.8388E-01 -9.4226E+03 SER
 FE                       9.3131E-01  9.7500E-01 8.2599E-03 -3.5891E+04 SER
 MN                       2.4275E-02  2.5000E-02 9.2895E-05 -6.9473E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 8.2303E-01, Mass 4.5951E+01, Volume fraction 8.4971E-01  Mass fractions:
 FE  9.93109E-01  MN  6.84649E-03  C   4.43634E-05

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.7697E-01, Mass 7.9271E+00, Volume fraction 1.5029E-01  Mass fractions:
 FE  8.04416E-01  MN  1.28547E-01  C   6.70366E-02
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    900.000     for:
     CEMENTITE
     FCC_A1
   9.000000E+02    0.932    0.068   2.565450E-02   3.333333E-01  -1.153988E+00
   8.900000E+02    0.929    0.071   2.464591E-02   3.333333E-01  -1.126046E+00
   8.800000E+02    0.926    0.074   2.365342E-02   3.333333E-01  -1.097677E+00
   8.700000E+02    0.923    0.077   2.267731E-02   3.333333E-01  -1.068876E+00
   8.600000E+02    0.921    0.079   2.171787E-02   3.333333E-01  -1.039637E+00
   8.500000E+02    0.918    0.082   2.077542E-02   3.333333E-01  -1.009957E+00
   8.400000E+02    0.915    0.085   1.985029E-02   3.333333E-01  -9.798293E-01
   8.300000E+02    0.912    0.088   1.894280E-02   3.333333E-01  -9.492495E-01
   8.200000E+02    0.910    0.090   1.805298E-02   3.333333E-01  -9.182117E-01
   8.100000E+02    0.907    0.093   1.718184E-02   3.333333E-01  -8.867123E-01
   8.000000E+02    0.905    0.095   1.632945E-02   3.333333E-01  -8.547455E-01

 Phase Region from    900.000     for:
     CEMENTITE
     FCC_A1
   9.000000E+02    0.932    0.068   2.565450E-02   3.333333E-01  -1.153988E+00
   9.100000E+02    0.935    0.065   2.667892E-02   3.333333E-01  -1.181507E+00
   9.200000E+02    0.939    0.061   2.771893E-02   3.333333E-01  -1.208608E+00
   9.300000E+02    0.942    0.058   2.877428E-02   3.333333E-01  -1.235296E+00
   9.400000E+02    0.945    0.055   2.984477E-02   3.333333E-01  -1.261574E+00
   9.500000E+02    0.949    0.051   3.093019E-02   3.333333E-01  -1.287449E+00
   9.600000E+02    0.952    0.048   3.203035E-02   3.333333E-01  -1.312923E+00
   9.700000E+02    0.956    0.044   3.314509E-02   3.333333E-01  -1.338002E+00
   9.800000E+02    0.959    0.041   3.427426E-02   3.333333E-01  -1.362689E+00
   9.900000E+02    0.963    0.037   3.541771E-02   3.333333E-01  -1.386988E+00
   1.000000E+03    0.967    0.033   3.657533E-02   3.333333E-01  -1.410903E+00
   1.010000E+03    0.970    0.030   3.774701E-02   3.333333E-01  -1.434438E+00
   1.020000E+03    0.974    0.026   3.893266E-02   3.333333E-01  -1.457597E+00
   1.030000E+03    0.978    0.022   4.013221E-02   3.333333E-01  -1.480383E+00
   1.040000E+03    0.982    0.018   4.134559E-02   3.333333E-01  -1.502799E+00
   1.050000E+03    0.987    0.013   4.257277E-02   3.333333E-01  -1.524850E+00
   1.060000E+03    0.991    0.009   4.381371E-02   3.333333E-01  -1.546538E+00
   1.070000E+03    0.995    0.005   4.506839E-02   3.333333E-01  -1.567866E+00
   1.080000E+03    1.000    0.000   4.633682E-02   3.333333E-01  -1.588838E+00
   1.090000E+03    1.004   -0.004   4.761901E-02   3.333333E-01  -1.609456E+00
   1.100000E+03    1.009   -0.009   4.891498E-02   3.333333E-01  -1.629723E+00
   1.110000E+03    1.013   -0.013   5.022479E-02   3.333333E-01  -1.649641E+00
   1.120000E+03    1.018   -0.018   5.154847E-02   3.333333E-01  -1.669214E+00
   1.130000E+03    1.023   -0.023   5.288611E-02   3.333333E-01  -1.688443E+00
   1.140000E+03    1.028   -0.028   5.423778E-02   3.333333E-01  -1.707332E+00
   1.150000E+03    1.033   -0.033   5.560358E-02   3.333333E-01  -1.725881E+00
   1.160000E+03    1.038   -0.038   5.698363E-02   3.333333E-01  -1.744093E+00
   1.170000E+03    1.043   -0.043   5.837804E-02   3.333333E-01  -1.761970E+00
   1.180000E+03    1.049   -0.049   5.978696E-02   3.333333E-01  -1.779514E+00
   1.190000E+03    1.054   -0.054   6.121053E-02   3.333333E-01  -1.796726E+00
   1.200000E+03    1.060   -0.060   6.264893E-02   3.333333E-01  -1.813608E+00
 *** Buffer savend on file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex42\TCEX42~2.POL
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n Mass u-fraction C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-tit example 42d
   ... the command in full is SET_TITLE
POST: app-e n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST:
POST: app-e y tcex42
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.02
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 42e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

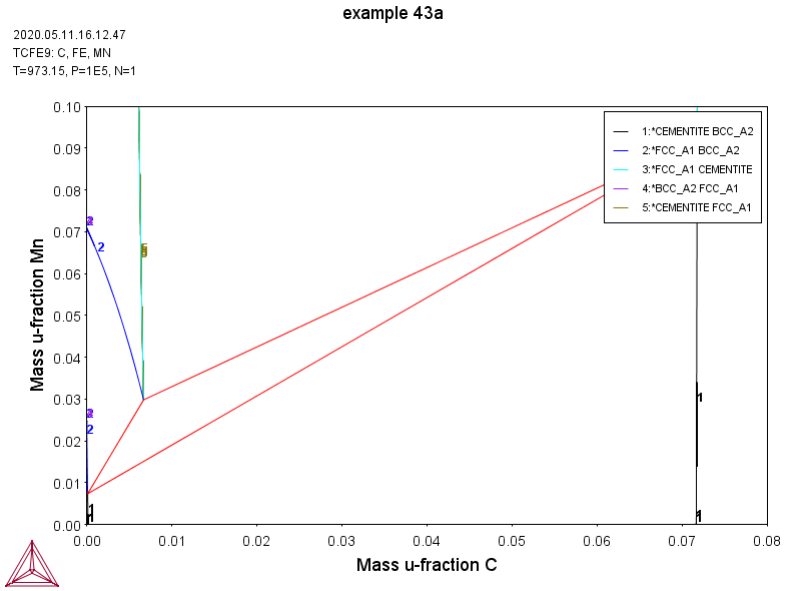
tcex43

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex43\tcex43.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Paraequilibrium calculation - Formation of
SYS: @@ Para-pearlite - Isothermal
SYS:
SYS: @@ This example uses an Fe-Mn-C system at 700 C to show a
SYS: @@ paraequilibrium calculation where there is formation of
SYS: @@ para-pearlite. It is an isothermal calculation and shows
SYS: @@ the Step_with_Options command.
SYS:
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex43,,,
SYS: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: d-mater
   ... the command in full is DEFINE_MATERIAL
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: tcfe9
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 0.1
2nd alloying element: mn 2
Next alloying element:
Temperature (C) /1000/: 700
 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
 REINITIATING GES .....
   ... the command in full is DEFINE_ELEMENTS
 FE  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 C  DEFINED
   ... the command in full is DEFINE_ELEMENTS
 MN  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           GRAPHITE
 CEMENTITE                M23C6                    M7C3
 M5C2                     KSI_CARBIDE              FE4N_LP1
 FECN_CHI                 LAVES_PHASE_C14          G_PHASE
 CUZN_EPSILON             AL5FE4                   FLUORITE_C1:I
 ZRO2_TETR:I              M2O3C:I                  M2O3H:I
Reject phase(s) /NONE/: graphite m5c2
 GRAPHITE                M5C2  REJECTED
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

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

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 FCC_A1                   HCP_A3                   CBCC_A12
 CUB_A13                  DIAMOND_FCC_A4           CEMENTITE
 M23C6                    M7C3                     KSI_CARBIDE
 FE4N_LP1                 FECN_CHI                 LAVES_PHASE_C14
 G_PHASE                  CUZN_EPSILON             AL5FE4
 FLUORITE_C1:I            ZRO2_TETR:I              M2O3C:I
 M2O3H:I

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

OK? /Y/: Y
16:12:36,319 INFO  *** Invoking Gibbs Energy System v6 ***
 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
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C as it has net charge
Suspending M2O3H as it has net charge
Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
```

```
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE9
      database (TCFE v9.0, Jan, 2017).'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'M. Seiersten, Unpublished work (1989); Al-Fe'
  'Unassessed parameter; Linear combination of unary data'
  '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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD,
      submitted, 2011; Fe-Mn-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'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279
      -85(2010); Mn-C'
  'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
  'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb
      and Fe-Mn-Nb'
  'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed
      solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the
      same phase as cubic Y2O3 (M2O3C).'
  'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114
      -21; Mn-Y-O'
  'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457
      -64; Mn-Zr-O, Mn-Y-Zr-O'
  'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE8
      database (TCFE v8, May, 2015).'
 -OK-
Should any phase have a miscibility gap check? /N/: N
 Using global minimization procedure
Calculated         17781 grid points in             2 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     2  s
POLY: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -4.11743E+04,  Enthalpy  2.45990E+04,  Volume  7.28130E-06

 Component                Moles       W-Fraction  Activity   Potential  Ref.stat
 C                        4.6312E-03  1.0000E-03 1.2686E-01 -1.6706E+04 SER
 FE                       9.7512E-01  9.7900E-01 6.6201E-03 -4.0599E+04 SER
 MN                       2.0250E-02  2.0000E-02 1.0065E-04 -7.4471E+04 SER

 BCC_A2                      Status ENTERED     Driving force  0.0000E+00
 Moles 7.8411E-01, Mass 4.3770E+01, Volume fraction 7.8786E-01  Mass fractions:
 FE  9.87020E-01  MN  1.29131E-02  C   6.70810E-05

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 2.1589E-01, Mass 1.1856E+01, Volume fraction 2.1214E-01  Mass fractions:
 FE  9.49391E-01  MN  4.61646E-02  C   4.44430E-03
POLY:

POLY: @@ Change the status of component C to SPECIAL and work
POLY: @@ with u-fractions
POLY: c-s comp c
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: spe
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY: s-a-v 1 w(c) 0 0.08
   ... the command in full is SET_AXIS_VARIABLE
Increment /.002/: 2.5E-04
POLY: s-a-v 2 w(mn) 0 0.1
   ... the command in full is SET_AXIS_VARIABLE
Increment /.0025/: .0025
POLY: 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: sa tcex43a y
   ... the command in full is SAVE_WORKSPACES
POLY: 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
```

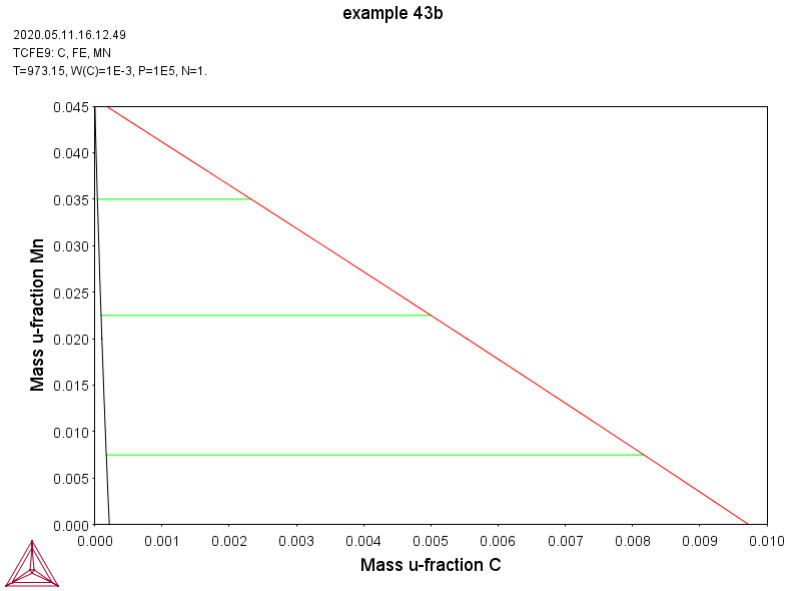
```
 Generating start equilibrium  8
 Generating start equilibrium  9
 Generating start equilibrium 10
 Generating start equilibrium 11
 Generating start equilibrium 12

 Organizing start points

Using ADDED start equilibria

 Working hard
 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
 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:   3.082E-02  1.597E-02
     BCC_A2
  ** CEMENTITE
 Calculated                      17 equilibria

 Phase region boundary   2 at:   3.082E-02  1.597E-02
     BCC_A2
  ** CEMENTITE
 Calculated.                      12 equilibria

 Phase region boundary   3 at:   3.082E-02  4.346E-02
     BCC_A2
  ** CEMENTITE
  ** FCC_A1

 Phase region boundary   4 at:   3.349E-03  1.844E-02
     BCC_A2
  ** FCC_A1
 Calculated                      33 equilibria

 Phase region boundary   5 at:   3.506E-02  5.674E-02
     CEMENTITE
  ** FCC_A1
 Calculated..                      48 equilibria
 Terminating at axis limit.

 Phase region boundary   6 at:   3.082E-02  4.346E-02
     BCC_A2
  ** CEMENTITE
 Calculated                      27 equilibria

 Phase region boundary   7 at:   3.082E-02  1.597E-02
     BCC_A2
  ** CEMENTITE
 Calculated                      17 equilibria

 Phase region boundary   8 at:   3.082E-02  1.597E-02
     BCC_A2
  ** CEMENTITE
 Calculated.                      12 equilibria
 Terminating at known equilibrium

 Phase region boundary   9 at:   3.082E-02  2.819E-03
     BCC_A2
  ** CEMENTITE
 Calculated                      12 equilibria

 Phase region boundary  10 at:   3.082E-02  2.819E-03
     BCC_A2
  ** CEMENTITE
 Calculated.                      18 equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   3.082E-02  1.539E-03
     BCC_A2
  ** CEMENTITE
 Calculated                      13 equilibria

 Phase region boundary  12 at:   3.082E-02  1.539E-03
     BCC_A2
  ** CEMENTITE
 Calculated.                      18 equilibria
 Terminating at known equilibrium

 Phase region boundary  13 at:   4.555E-04  4.440E-02
     BCC_A2
  ** FCC_A1
 Calculated.                      18 equilibria
 Terminating at known equilibrium

 Phase region boundary  14 at:   4.555E-04  4.440E-02
     BCC_A2
  ** FCC_A1
 Calculated                      11 equilibria

 Phase region boundary  15 at:   1.376E-04  4.678E-02
  ** BCC_A2
     FCC_A1
 Calculated.                      19 equilibria
 Terminating at known equilibrium
```

```
 Phase region boundary  16 at:   1.376E-04  4.678E-02
  ** BCC_A2
     FCC_A1
 Calculated                     23 equilibria

 Phase region boundary  17 at:   3.478E-02  1.686E-01
  ** CEMENTITE
     FCC_A1
 Calculated.                     46 equilibria
 Terminating at known equilibrium

 Phase region boundary  18 at:   3.478E-02  1.686E-01
  ** CEMENTITE
     FCC_A1
 Calculated..                      3 equilibria
 Terminating at axis limit.

 Phase region boundary  19 at:   3.478E-02  1.711E-01
  ** CEMENTITE
     FCC_A1
 Calculated.                     47 equilibria
 Terminating at known equilibrium

 Phase region boundary  20 at:   1.264E-04  4.686E-02
  ** BCC_A2
     FCC_A1
 Calculated                     10 equilibria

 Phase region boundary  21 at:   1.264E-04  4.686E-02
  ** BCC_A2
     FCC_A1
 Calculated.                     14 equilibria
 Terminating at known equilibrium

 Phase region boundary  22 at:   3.491E-02  1.118E-01
  ** CEMENTITE
     FCC_A1
 Calculated.                     24 equilibria
 Terminating at known equilibrium

 Phase region boundary  23 at:   3.491E-02  1.118E-01
  ** CEMENTITE
     FCC_A1
 Calculated..                     26 equilibria
 Terminating at axis limit.

 Phase region boundary  24 at:   3.478E-02  1.718E-01
  ** CEMENTITE
     FCC_A1
 Calculated.                     48 equilibria
 Terminating at known equilibrium

 Phase region boundary  25 at:   3.501E-02  7.506E-02
  ** CEMENTITE
     FCC_A1
 Calculated.                      9 equilibria
 Terminating at known equilibrium

 Phase region boundary  26 at:   3.501E-02  7.506E-02
  ** CEMENTITE
     FCC_A1
 Calculated..                     40 equilibria
 Terminating at axis limit.

 Phase region boundary  27 at:   3.478E-02  1.701E-01
  ** CEMENTITE
     FCC_A1
 Calculated.                     47 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex43\tcex43a.POLY3
 CPU time for mapping                     8 seconds
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-lab e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 43a
POST: s-ax-text x N Mass u-fraction C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N Mass u-fraction Mn
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

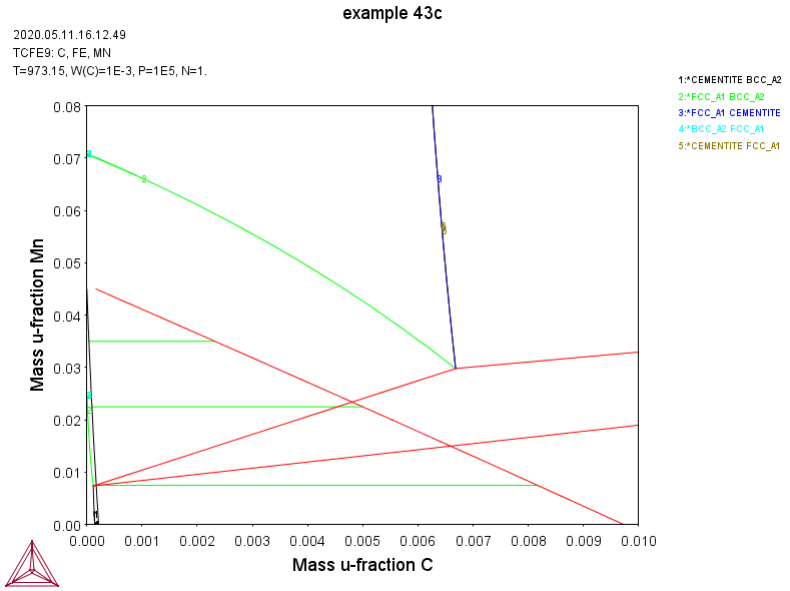



```
POST:
POST:Hit RETURN to continue
POST:
POST: make tcex43 y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: b
   ... the command in full is BACK
POLY: read tcex43a
   ... the command in full is READ_WORKSPACES
POLY: s-a-v 1 w(mn) 0 0.1
   ... the command in full is SET_AXIS_VARIABLE
Increment /.0025/: .0025
POLY: s-a-v 2 none
   ... the command in full is SET_AXIS_VARIABLE
POLY: sa tcex43b y
   ... the command in full is SAVE_WORKSPACES
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from   0.200000E-01 for:
     BCC_A2
     FCC_A1
   2.000000E-02    0.165    0.835   2.571917E-02   4.926111E-04  -1.658124E+00
   1.750000E-02    0.148    0.852   2.818430E-02   5.501151E-04  -1.529395E+00
   1.500000E-02    0.134    0.866   3.064279E-02   6.094293E-04  -1.408661E+00
   1.250000E-02    0.123    0.877   3.309442E-02   6.705749E-04  -1.294692E+00
   1.000000E-02    0.112    0.888   3.553901E-02   7.335731E-04  -1.186526E+00
   7.500000E-03    0.104    0.896   3.797641E-02   7.984452E-04  -1.083396E+00
   5.000000E-03    0.096    0.904   4.040649E-02   8.652122E-04  -9.846802E-01
   2.500000E-03    0.089    0.911   4.282917E-02   9.338953E-04  -8.898660E-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   2.571917E-02   4.926111E-04  -1.658124E+00
   2.250000E-02    0.185    0.815   2.324766E-02   4.368958E-04  -1.796453E+00
   2.500000E-02    0.209    0.791   2.077008E-02   3.829481E-04  -1.946535E+00
   2.750000E-02    0.240    0.760   1.828677E-02   3.307465E-04  -2.111350E+00
   3.000000E-02    0.281    0.719   1.579818E-02   2.802698E-04  -2.295199E+00
   3.250000E-02    0.338    0.662   1.330418E-02   2.314911E-04  -2.504641E+00
   3.500000E-02    0.420    0.580   1.080635E-02   1.843977E-04  -2.750300E+00
   3.750000E-02    0.552    0.448   8.304909E-03   1.389646E-04  -3.051369E+00
   4.000000E-02    0.798    0.202   5.800616E-03   9.517043E-05  -3.448092E+00
   4.250000E-02    1.418   -0.418   3.294358E-03   5.299403E-05  -4.051736E+00
   4.500000E-02    5.984   -4.984   7.871561E-04   1.241421E-05  -5.521207E+00
 *** Buffer savend on file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex43\TCEX43~2.POL
 *** ERROR     7 IN NS01AD: Numerical error
POLY: po
   ... the command in full is POST
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y w(*,mn)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 43b
POST: s-ax-text x N Mass u-fraction C
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N Mass u-fraction Mn
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
```

```
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



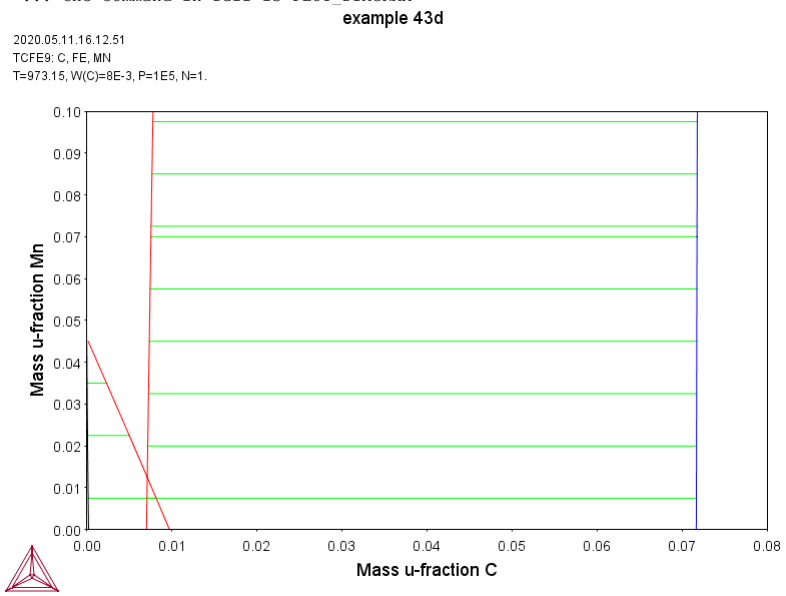

```
POST:
POST:Hit RETURN to continue
POST:
POST: app y tcex43
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.01
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.08
   ... the command in full is SET_SCALING_STATUS
POST: set-title example 43c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



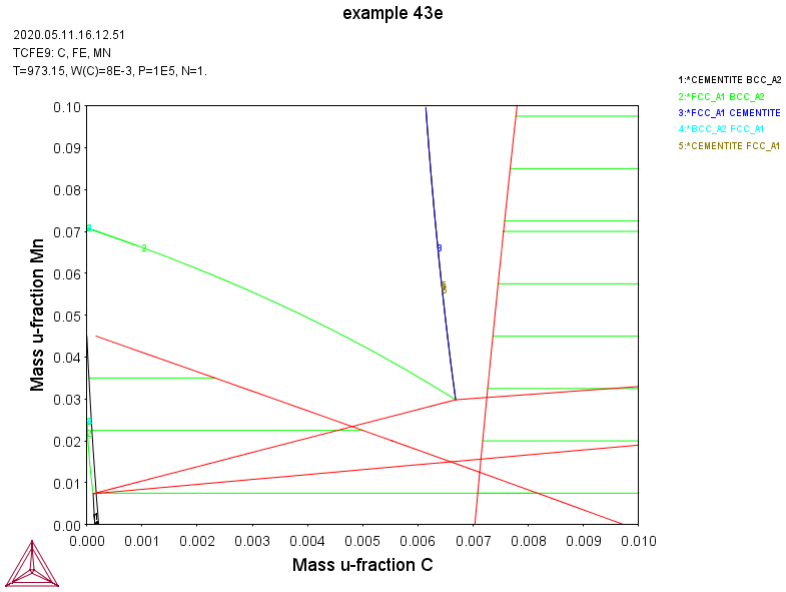

```
POST:
POST:Hit RETURN to continue
POST:
POST: b
   ... the command in full is BACK
POLY: read tcex43b
   ... the command in full is READ_WORKSPACES
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 T=973.15, W(C)=1E-3, W(MN)=2E-2, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY: s-c w(c)=0.008 w(mn)=0.07
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         17781 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
```

```
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -4.19930E+04,  Enthalpy  2.75209E+04,  Volume  7.10744E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       3.5823E-02  8.0000E-03 1.7545E-01 -1.4082E+04 SER
 FE                      8.9565E-01  9.3000E-01 6.4327E-03 -4.0831E+04 SER
 MN                      6.8530E-02  7.0000E-02 1.4064E-04 -7.1764E+04 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 9.6764E-01, Mass 5.2766E+01, Volume fraction 9.7258E-01  Mass fractions:
 FE  9.27199E-01  MN  6.64886E-02  C   6.31288E-03

 CEMENTITE                   Status ENTERED     Driving force  0.0000E+00
 Moles 3.2359E-02, Mass 1.4483E+00, Volume fraction 2.7422E-02  Mass fractions:
 FE  7.55773E-01  MN  1.77136E-01  C   6.70903E-02
POLY: advanced
   ... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 NP(FCC_A1) =   0.9930 with U-fractions C  =  3.50620E-02
 NP(CEMENTITE) =   0.0070 with U-fractions C  =  3.33333E-01
 All other compositions the same in both phases
 Note: LIST-EQUILIBRIUM is not relevant
POLY: step
   ... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from   0.700000E-01 for:
     CEMENTITE
     FCC_A1
   7.000000E-02    0.993    0.007   3.506202E-02   3.333333E-01  -1.531041E+00
   6.750000E-02    0.993    0.007   3.497163E-02   3.333333E-01  -1.520671E+00
   6.500000E-02    0.992    0.008   3.488168E-02   3.333333E-01  -1.510310E+00
   6.250000E-02    0.992    0.008   3.479215E-02   3.333333E-01  -1.499958E+00
   6.000000E-02    0.992    0.008   3.470304E-02   3.333333E-01  -1.489616E+00
   5.750000E-02    0.991    0.009   3.461436E-02   3.333333E-01  -1.479282E+00
   5.500000E-02    0.991    0.009   3.452609E-02   3.333333E-01  -1.468959E+00
   5.250000E-02    0.991    0.009   3.443825E-02   3.333333E-01  -1.458644E+00
   5.000000E-02    0.991    0.009   3.435082E-02   3.333333E-01  -1.448340E+00
   4.750000E-02    0.990    0.010   3.426423E-02   3.333333E-01  -1.438045E+00
   4.500000E-02    0.990    0.010   3.417757E-02   3.333333E-01  -1.427759E+00
   4.250000E-02    0.990    0.010   3.409132E-02   3.333333E-01  -1.417483E+00
   4.000000E-02    0.989    0.011   3.400550E-02   3.333333E-01  -1.407216E+00
   3.750000E-02    0.989    0.011   3.392009E-02   3.333333E-01  -1.396959E+00
   3.500000E-02    0.989    0.011   3.383510E-02   3.333333E-01  -1.386712E+00
   3.250000E-02    0.989    0.011   3.375052E-02   3.333333E-01  -1.376474E+00
   3.000000E-02    0.988    0.012   3.366635E-02   3.333333E-01  -1.366246E+00
   2.750000E-02    0.988    0.012   3.358258E-02   3.333333E-01  -1.356028E+00
   2.500000E-02    0.988    0.012   3.349923E-02   3.333333E-01  -1.345820E+00
   2.250000E-02    0.988    0.012   3.341628E-02   3.333333E-01  -1.335622E+00
   2.000000E-02    0.987    0.013   3.333373E-02   3.333333E-01  -1.325434E+00
   1.750000E-02    0.987    0.013   3.325158E-02   3.333333E-01  -1.315255E+00
   1.500000E-02    0.987    0.013   3.316983E-02   3.333333E-01  -1.305087E+00
   1.250000E-02    0.986    0.014   3.308848E-02   3.333333E-01  -1.294928E+00
   1.000000E-02    0.986    0.014   3.300753E-02   3.333333E-01  -1.284780E+00
   7.500000E-03    0.986    0.014   3.292696E-02   3.333333E-01  -1.274642E+00
   5.000000E-03    0.986    0.014   3.284679E-02   3.333333E-01  -1.264514E+00
   2.500000E-03    0.985    0.015   3.276701E-02   3.333333E-01  -1.254396E+00
   2.500000E-09    0.985    0.015   3.268761E-02   3.333333E-01  -1.244288E+00

 Phase Region from   0.700000E-01 for:
     CEMENTITE
     FCC_A1
   7.000000E-02    0.993    0.007   3.506202E-02   3.333333E-01  -1.531041E+00
   7.250000E-02    0.993    0.007   3.515283E-02   3.333333E-01  -1.541421E+00
   7.500000E-02    0.994    0.006   3.524407E-02   3.333333E-01  -1.551809E+00
   7.750000E-02    0.994    0.006   3.533574E-02   3.333333E-01  -1.562207E+00
   8.000000E-02    0.994    0.006   3.542785E-02   3.333333E-01  -1.572614E+00
   8.250000E-02    0.995    0.005   3.552039E-02   3.333333E-01  -1.583030E+00
   8.500000E-02    0.995    0.005   3.561338E-02   3.333333E-01  -1.593455E+00
   8.750000E-02    0.995    0.005   3.570680E-02   3.333333E-01  -1.603888E+00
   9.000000E-02    0.995    0.005   3.580066E-02   3.333333E-01  -1.614331E+00
   9.250000E-02    0.996    0.004   3.589497E-02   3.333333E-01  -1.624783E+00
   9.500000E-02    0.996    0.004   3.598972E-02   3.333333E-01  -1.635243E+00
   9.750000E-02    0.996    0.004   3.608492E-02   3.333333E-01  -1.645712E+00
   1.000000E-01    0.997    0.003   3.618056E-02   3.333333E-01  -1.656190E+00
 *** Buffer savend on file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex43\TCEX43~2.POL
POLY: po
   ... the command in full is POST
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x w(*,c)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y w(*,mn)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-tie 5
   ... the command in full is SET_TIELINE_STATUS
POST: set-title example 43d
POST: s-ax-text x N Mass u-fraction C
```

```
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N Mass u-fraction Mn
   ... the command in full is SET_AXIS_TEXT_STATUS
POST: app-e n
   ... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:Hit RETURN to continue
POST:
POST: s-s x n 0 0.01
   ... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.10
   ... the command in full is SET_SCALING_STATUS
POST: app-e y tcex43
   ... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 43e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex44

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex44\tcex44.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Exploring variables and functions.
SYS:
SYS: @@ This example uses variables and functions to predict
SYS: @@ properties e.g. proof strength for an austenitic
SYS: @@ stainless steel at elevated temperatures (20-550 C).
SYS: @@ The example was created using an expression from
SYS: @@ Eliasson, J., and SandstrÃ¶m, R. (2000). 'Proof
SYS: @@ strength values for austenitic stainless steels at
SYS: @@ elevated temperatures', Steel Research, 71(6â€"7), 249â€"254.
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: go da
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw tcfe9
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9: def-sys
ELEMENTS: fe c si mn cr ni mo cu n
 FE                      C                       SI
 MN                      CR                      NI
 MO                      CU                      N
   DEFINED
TDB_TCFE9: get
16:14:09,361 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 Creating a new composition set HCP_A3#2
Suspending FLUORITE_C1 as it has net charge
Suspending M2O3C as it has net charge
Suspending M2O3H as it has net charge
Suspending ZRO2_TETR as it has net charge
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
  'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.-J. Lee, KRISS, Unpublished research, during 1993-1995'
  'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE9
      database (TCFE v9.0, Jan, 2017).'
  'N. Saunders, COST 507 Report (1998); Al-Cu'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2012; Molar volumes'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'N. Saunders, COST 507 Report (1998); Mn-Ti'
  'W. Zheng, J. Alloys Compd., 632 (2015) 661-675'
  'J-O. Andersson, CALPHAD, 12 (1988) 1-8; TRITA 0317 (1986); C-MO'
  'Unassessed parameter; Linear combination of unary data'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'A. Fernandez Guillermet, Z. Metallkd., 79 (1988) 524-536, TRITA-MAC 362
      (1988); C-CO-NI AND C-CO-FE-NI'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES_PHASE_C14'
  'I. Ansara, Unpublished work (1991); Cr-Si'
  'M. Seiersten, Unpublished work (1989); Al-Fe'
  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C-Cr-Nb'
  'J-O. Andersson, CALPHAD, 11 (1987) 271-276; TRITA 0314; C-CR'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'B.-J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'C. Qiu, ISIJ International, 32 (1992) 1117-1127; C-Cr-Fe-Mo'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  '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.-J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  'P. Gustafson, Inst. Met. Res. (IM-2549, 1990); C-CU-FE'
  'Chandrakasekan et. al, (1987) provisional; CU-FE-P-C'
  '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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C-FE-MO'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
```

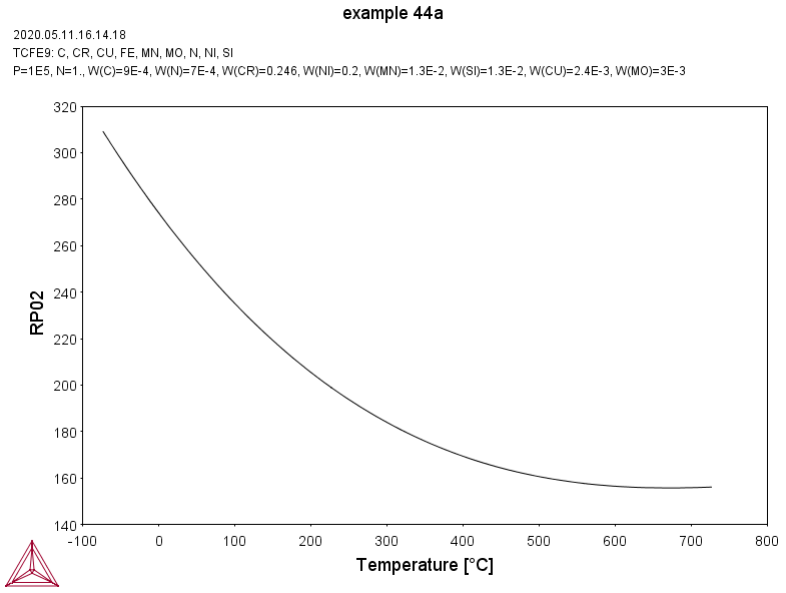
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, submitted, 2011; Fe-Mn-C'
'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev 1989); C-FE-MN'
'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, CALPHAD, 34, 279 -85(2010); Mn-C'
'J.-H. Shim, C.-S. Oh, D.N. Lee, Metall. Mater. Trans. B. 27 (1996) 955 -966; Ti-Mo-C'
'Thermo-Calc Software, Sweden, 2019: Volume data updated for TCFE9 database (TCFE v9.1, June, 2019).'
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci. (Parameters listed in CALPHAD, 11 (1987) 203-218); C-NI'
'A. Gabriel, P. Gustafson, and I. Ansara, CALPHAD, 11 (1987) 203-218; TRITA-MAC 285 (1986); C-FE-NI'
'A. Fernandez Guillermet and G. Grimvall,J. Phys. Chem. Solids, 1992, 53, 105-125; Molar volumes'
'J. Grobner, H.L. Lukas and F. Aldinger, CALPHAD, 20 (1996) 247-254; Si-C and Al-Si-C'
'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991) 2211-2223; Fe-Si and Fe-Si-C'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
'Thermo-Calc Software, Sweden, 2008: Volume data updated for TCFE6 database (TCFE v6, April, 2008).'
'NPL, Unpublished work (1989); C-Mn-Si'
'W. Xiong, Y. Du, X. Lu, J.C. Schuster, H. Chen, Intermetallics. 15 (2007) 1401-1408.'
'H. Wang, Z. Li, Z. Chen, B. Yang, J. Phase Equilib. Diffus. 37 (2016) 1-7'
'K. Zeng and M. Hamalainen, CALPHAD, 19 (1995) 93-104; Cr-Cu'
'B. Sundman, Private communication, 2(1999); Estimated parameter'
'COST2 database 1997'
'W.H. Sun, S.H. Liu, added to make this phase less stable, 2010'
'B.-J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe-Ni liquid'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270 (1986); CR-FE'
'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR -FE-N'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986); CR-FE-MO'
'B.-J. Lee, Private communication, (1999); Estimated parameter'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Cr-Fe-Zn'
'Thermo-Calc Software, Sweden, 2014: Volume data updated for TCFE8 database (TCFE v8, May, 2015).'
'B.-J. Lee, Metall. Trans. A, 24A (1993) 1919-1933; Cr-Mn, Fe-Cr-Mn'
'K. Frisk, CALPHAD, 17 (1993) 335-349; Cr-Mn-N'
'SGTE (2008): SSOL4 - SGTE Substance Database V4.1, provided by Thermo -Calc Software'
'K. Frisk, KTH Report D 60 (1984); CR-MO'
'B. Sundman, Private communication; FCC parameter same as BCC; Cr-Mo'
'J-O. Andersson, TRITA-MAC 323 (1986); C-CR-FE-MO'
'K. Frisk, TRITA-MAC 429 (1990); CR-MO-NI'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2015; LAVES_PHASE_C14'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Z_PHASE'
'K. Frisk, CALPHAD, 15 (1991) 79-106; TRITA-MAC 393 (1989); CR-N, FE-N, MO -N, CR-MO-N'
'Estimated parameter for solubility of N in cementite, 1999'
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Reassessed solubility of Al, Cr, Fe, Ni in Mn2O3. When Mn2O3 is modelled as the same phase as cubic Y2O3 (M2O3C).'
'A. Jacob, E. Povoden-Karadeniz, E. Kozeschnik, Calphad, 56 (2017) 80-91.'
'I. Ansara and A. Jansson, TRITA-MAC 533 (1993); Cu-Fe'
'C.Y. He, J. Alloys Compd.,457,233-238 (2008); Cu-Mn'
'C.P. Wang, X.J. Liu, I. Ohnuma, R. Kainuma, K. Ishida, S.M. Hao, J. Phase Equilib. Diffus. 21 (2000) 54-62; Cu-Mo and Cu-Fe-Mo'
'Same or similar interaction as in the corresponding stable phase'
'K. Frisk, IM-2929, Swedish Inst. Met. Res., (1992); Cu-N, Fe-Cu-N'
'S. an Mey, CALPHAD, 16 (1992) 255-260; Cu-Ni'
'A. Jansson, TRITA-MAC 340 (1987); CU-FE-NI'
'M. Jacobs (1991), Revised by T. Buehler (1997), COST 507 Report; Cu-Si'
'S.G.Fries, H.L. Lukas, R. Konetzki, R. Schimd-Fetzer, J. Phase Equilib., 15 (1994) 606-614; Cu-Y'
'H. Mao, Thermo-Calc Software AB, Sweden, 2013; Molar volumes'
'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Unifying HCP_ZN with HCP_A3'
'W. Huang, CALPHAD, 13 (1989) 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'S. Liu, B. Hallstedt, D. Music, Y. Du, CALPHAD, 38 (2012) 43-58; Mn-Nb and Fe-Mn-Nb'
'A. Markstrom, Thermo-Calc software AB, Sweden, 2011'
'A. Fernandez Guillermet, CALPHAD, 6 (1982) 127-140; (sigma phase revised 1986); TRITA-MAC 200 (1982); FE-MO'
'K. Frisk, TRITA-MAC 428 (1990); FE-MO-NI'
'H.K. Danielsen and J. Hald, CALPHAD, 31 (2007) 505-514; Z-PHASE'
'C. Qiu, Metall. Trans. A, 24A (1993) 629-645; Fe-Mn-N'
'A. Dinsdale, T. Chart, MTDS NPL, Unpublished work (1986); FE-NI'
'L. Zhang, Y. Du, H. Xu, S. Liu, Y. Liu, F. Zheng, et al., Int. J. Mater. Res. 100 (2009) 160-175; Fe-Mn-Ni'
'J. Miettinen and B. Hallstedt, CALPHAD, 22 (1998) 231-256; Fe-Si and Fe -Si-C'
'S. Cotes, A.F. Guillermet, M. Sade, J. Alloys Compd., 208(1998) 168-177'
'A. Forsberg and J. Agren, J. Phase Equilib., 14 (1993) 354-363; Fe-Mn-Si'
'C. Qiu and A. Fernandez Guillermet, Z. Metallkd., 84 (1993) 11-12; Mn-N'
'A. Markstrom, Thermo-Calc Software AB, Sweden, 2010; Molar volumes'
'S. Liu, Unpublished work (2010); Mn-Ni'
'C.P. Guo,Intermetallics,13(5),525-534,(2005); Mn-Ni'
'M. Chen, B. Hallstedt, L. J. Gauckler, J. Alloys Compd., 393 (2005) 114 -21; Mn-Y-O'
'M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 176 (2005) 1457 -64; Mn-Zr-O, Mn-Y-Zr-O'
'J. Miettinen, CALPHAD, 28 (2004) 313-320; Mn-Zn'
'K. Frisk and B. Uhrenius, Metall. Mater. Trans. A, 27A (1996) 2869-2880; Mo-C-N, Fe-Mo-C-N'
'K. Frisk, CALPHAD, 14 (1990) 311-320; MO-NI'
'Y. Liu, G. Shao, P. Tsakiropoulos, Intermatallics 8 (2000) 953-962; Mo-Si, Al-Mo-Si'
'A. Kusoffsky et al., Work within CCT-Applied Stainless steels, 2004; Fe -Cr-Si, Fe-Ni-Si, Fe-Cr-Cu, Fe-Cu-Mo, Cr-Mo-N-Ni, Fe-Cr-N-Ni, Fe-Al-Cr -Ni'
'K. Frisk, Z. Metallkd., 82 (1991) 59-66; TRITA-MAC 414 (1989); Fe-Ni-N'
'K. Frisk, Int. J. Thermophys., 12 (1990) 417-431; TRITA-MAC 419 (1990); N -NI'
'X. Ma, C. Li, F. Wang, W. Zhang, CALPHAD, 27 (2003) 383-388; N-Si'
'P. Gustafson, Inst. Met. Res. (Sweden) (1990); Estimations of C-CR-FE-V, C-CR-FE-MO-V-W, FE-N-W, FE-MN-N, FE-N-SI, CR-N-V, C-CR-N, FE-MO-N, CR

```
     -N-W, CR-TI-N'
  'Thermo-Calc Software, Sweden, 2009: Volume data updated for TCFE6
     database (TCFE v6, November, 2009).'
  'A. Bolcavage and U.R. Kattner, J. Phase Equilib., 2, (1996); Nb-Ni'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden, 2013; Estimated parameter;
      Ni-Zr-O'
  'P. Bellen, K.C. Hari Kumar and P. Wollants, Z. Metallkd., 87 (1994) 972
     -978; Ni-Ti'
  'J. Miettinen, CALPHAD, 27 (2003) 263-274; Cu-Ni-Zn'
  'H.Liang, Y.A.Chang, J. Phase Equilib. 19 (1998) 25-37'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24-33(2014); Cr-Fe-C'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
     -CR-FE'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Fe-Cr-Mo-V-W-C'
  'NPL, Unpublished work (1989); C-Cr-Ni'
  'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; C-Cr-Si'
  'S. Nagakura, Transactions of the Iron and Steel Institute of Japan, 8
     (1968) 265-294; Molar volumes'
  'I.K. Kupalova, V.I. Pavlova, High Speed Steels: Physical Properties,
     Prop. Data Updat. 2 (1988) 67-78; Molar volumes'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2014; Revision of the liquid
     C-Fe-Si description'
  'W. Zheng et al., J. Iron Steel Res. Int. 24(2)(2017) 190-197'
  'C.P. Wang, D.X. Huang, J.J. Zhu, S.Y. Yang, X.J. Liu, J. Phase Equilib.
     Diffus. 35 (2014) 314-325; Cr-Cu-Mo and Cr-Cu-W'
  'T. Ikoma, M. Kajihara, Mater. Sci. Eng. A. 437 (2006) 293-300; Cr-Cu-Ni'
  'C. Qiu, Metall. Trans. A, 24A (1993) 2393-2409; Cr-Fe-Mn-N'
  'A. Markstrom, Thermo-Calc Software AB, Sweden, 2013; Extrapolations,
     assumptions and adjustment'
  'B. Sundman, Private communication, (2000); Estimated Cr-Ni-Mo'
  'B.-J. Lee, Private communication, (2000); Estimated parameter'
  'A. Kusoffsky, Work within CCT-Applied Stainless steels, 2003; Fe-Cr-N, Fe
     -C-Cr-N, Fe-Cr-Mo-N, Fe-Cr-Mn-N'
  'K. Frisk, TRITA-MAC 422 (1990); CR-FE-N-NI'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Fe-Cr-Ni'
  'J. Miettinen, CALPHAD, 23 (2)(1999) 249-262; Cr-Fe-Si'
  'L. Zhang, Y. Du, Q. Chen, H. Xu, F. Zheng, C. Tang, H. Chen, Int. J.
     Mater. Res. 99 (2008) 1306-1318; Cu-Fe-Mn'
  'J. Miettinen, CALPHAD, 27 (2003) 389-394, Cu-Fe-Si'
  'W.H. Sun, CALPHAD, 33 (2009) 642-649; Cu-Mn-Ni'
  'K. Frisk, TRITA-MAC 433 (1990); FE-CR-MO-NI-N'
  'J. Miettinen, CALPHAD, 22 (1998) 275-300; Fe-Mo-Si'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Fe-Nb-Si'
  'J. Miettinen, G. Vassilev, J. Phase Equilib. Diffus, 37(5) 2016, 283-290;
     Fe-P-Si'
  'B. Hu, Unpublished (2010); Mn-Ni-Si,Al-Cu-Fe-Ni'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Carbonitrides and
     M23C6'
  'J. Bratberg, Thermo-Calc Software AB, Sweden, 2008; Solubilities in M6C'
 -OK-
TDB_TCFE9:
TDB_TCFE9: go p-3

 POLY version  3.32
POLY:

POLY: s-c p=1e5,n=1,t=1353
POLY: s-c w(c)=0.0009,w(n)=0.0007,w(cr)=.246,w(ni)=0.2,w(mn)=0.013
POLY: s-c w(si)=0.013,w(cu)=0.0024,w(mo)=0.003
POLY: 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: c-e
 Using global minimization procedure
Calculated         37553 grid points in             3 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       2 s, total time     5  s
POLY: l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -8.11349E+04,  Enthalpy  3.59560E+04,  Volume  7.33253E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.0809E-03  9.0000E-04 1.3103E-03 -7.4668E+04 SER
 CR                      2.5767E-01  2.4600E-01 2.7617E-03 -6.6281E+04 SER
 CU                      2.0569E-03  2.4000E-03 7.7572E-05 -1.0647E+05 SER
 FE                      5.0808E-01  5.2100E-01 1.1354E-03 -7.6281E+04 SER
 MN                      1.2887E-02  1.3000E-02 8.2607E-06 -1.3166E+05 SER
 MO                      1.7030E-03  3.0000E-03 6.1548E-05 -1.0907E+05 SER
 N                       2.7217E-03  7.0000E-04 1.5831E-07 -1.7615E+05 SER
 NI                      1.8559E-01  2.0000E-01 2.2490E-04 -9.4495E+04 SER
 SI                      2.5209E-02  1.3000E-02 3.4043E-08 -1.9344E+05 SER

 FCC_A1#1                     Status ENTERED     Driving force  0.0000E+00
 Moles 9.9137E-01, Mass 5.4075E+01, Volume fraction 9.9241E-01  Mass fractions:
 FE  5.23621E-01  NI  2.01292E-01  MN  1.30471E-02  CU  2.41718E-03  C   5.09797E-04
 CR  2.42476E-01  SI  1.30930E-02  MO  2.83895E-03  N   7.05010E-04

 M23C6                        Status ENTERED     Driving force  0.0000E+00
 Moles 8.6311E-03, Mass 3.8703E-01, Volume fraction 7.5879E-03  Mass fractions:
 CR  7.38318E-01  C   5.54188E-02  NI  1.95382E-02  N   0.00000E+00  SI  0.00000E+00
 FE  1.54808E-01  MO  2.55018E-02  MN  6.41532E-03  CU  0.00000E+00
POLY:
POLY: @@ Define some variables
POLY: enter-symb
Constant, variable, function or table? /FUNCTION/: variable
Name: cc
Function: 100*w(fcc_a1,c)
&
POLY: ent var csi=100*w(fcc_a1,si);
POLY: ent var cmn=100*w(fcc_a1,mn);
POLY: ent var ccr=100*w(fcc_a1,cr);
POLY: ent var cni=100*w(fcc_a1,ni);
POLY: ent var cmo=100*w(fcc_a1,mo);
```

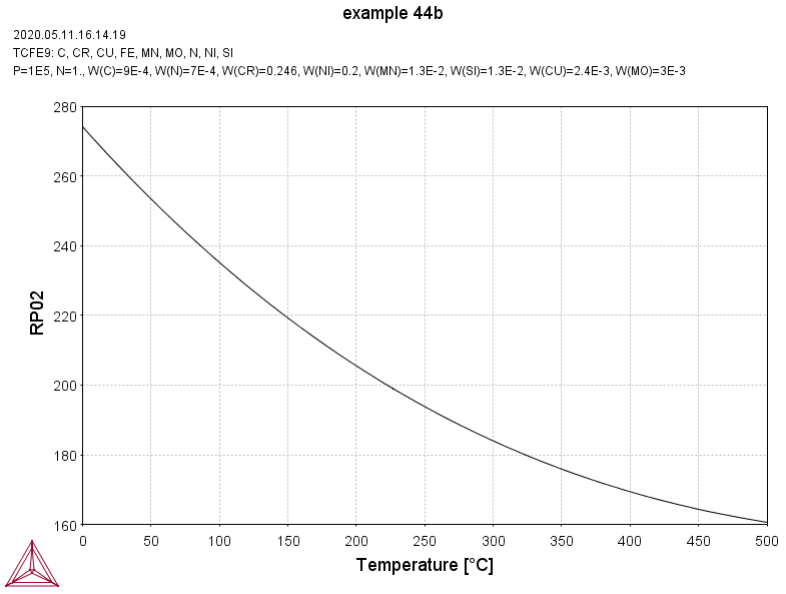
```
POLY: ent var ccu=100*w(fcc_a1,cu);
POLY: ent var cn=100*w(fcc_a1,n);
POLY: ent var cfe=100*w(fcc_a1,fe);
POLY: ent var cm23=100*bpw(m23c6);
POLY:
POLY: li-sy
 DEFINED FUNCTIONS AND VARIABLES%
    CC%=100*W(FCC_A1#1,C)
    CSI%=100*W(FCC_A1#1,SI)
    CMN%=100*W(FCC_A1#1,MN)
    CCR%=100*W(FCC_A1#1,CR)
    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:
POLY: eval
Name(s): *
 CC=5.0979749E-2
 CSI=1.3093044
 CMN=1.3047128
 CCR=24.247638
 CNI=20.12916
 CMO=0.283895
 CCU=0.24171773
 CN=7.0501005E-2
 CFE=52.362091
 CM23=0.71063528
POLY:
POLY: enter-symb
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: tc=t-273.15;
POLY:
POLY: @@ Enter empirical parameters as function of temperature
POLY: ent func bc=575-0.3686*tc;
POLY: ent func bsi=24.76+1.129e-4*tc*tc-0.09*tc;
POLY: ent func bmn=-1.4-0.007*tc;
POLY: ent func bcr=0.3-tc*7e-4;
POLY: ent func bni=5.3-tc*3.3e-3;
POLY: ent func bmo=6-tc*3.3e-3;
POLY: ent func bcu=-14+0.0116*tc;
POLY: ent func bn=937-2.74e-6*tc*tc*tc+5.24e-3*tc*tc-3.08*tc;
POLY: ent func bm23=48+0.0135*tc;
POLY: ent func at=1.68+4.248e-6*tc*tc-4.33e-3*tc;
POLY:
POLY: 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:
POLY: eval
Name(s): *
 CC=5.0979749E-2
 CSI=1.3093044
 CMN=1.3047128
 CCR=24.247638
 CNI=20.12916
 CMO=0.283895
 CCU=0.24171773
 CN=7.0501005E-2
 CFE=52.362091
 CM23=0.71063528
 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:
POLY: @@ Enter an empirical expression for the proof strength
POLY: @@ combining the variables and function parameters
POLY: @@ previously entered.
POLY: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp1
Function: at+bc*cc+bsi*csi+bmn*cmn+bni*cni;
POLY:
POLY: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp2
Function: bcr*ccr+bmo*cmo+bcu*ccu+bn*cn+bm23*cm23;
POLY:
POLY: ent func rp02=rp1+rp2;
POLY:
POLY: eval
Name(s): *
 CC=5.0979749E-2
```

```
 CSI=1.3093044
 CMN=1.3047128
 CCR=24.247638
 CNI=20.12916
 CMO=0.283895
 CCU=0.24171773
 CN=7.0501005E-2
 CFE=52.362091
 CM23=0.71063528
 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=111.78638
 RP2=52.865977
 RP02=164.65236
POLY:
POLY: @@ Turn off the global minimization calculation and suspend
POLY: @@ all phases except fcc_a1#1. This speeds up the calculation
POLY: @@ and does not affect the results.
POLY: advanced
Which option? /STEP_AND_MAP/: glo
 Settings for global minimization:
   Use global minimization as much as possible /Y/: n,,,,
POLY:
POLY: c-s phase
Phase name(s): *
Status: /ENTERED/: sus
POLY:
POLY: c-s phase fcc_a1#1=enter 1
POLY:
POLY: s-c t=500
POLY: 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: l-e,,,
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE9

 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 -1.86546E+04,  Enthalpy  9.45115E+03,  Volume  7.00887E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       4.0809E-03  9.0000E-04 1.1335E-01 -9.0513E+03 SER
 CR                      2.5767E-01  2.4600E-01 2.3546E-01 -6.0122E+03 SER
 CU                      2.0569E-03  2.4000E-03 3.7195E-01 -4.1116E+03 SER
 FE                      5.0808E-01  5.2100E-01 3.3392E-02 -1.4132E+04 SER
 MN                      1.2887E-02  1.3000E-02 2.7741E-05 -4.3620E+04 SER
 MO                      1.7030E-03  3.0000E-03 6.3987E-02 -1.1429E+04 SER
 N                       2.7217E-03  7.0000E-04 5.3177E-14 -1.2707E+05 SER
 NI                      1.8559E-01  2.0000E-01 9.8313E-04 -2.8788E+04 SER
 SI                      2.5209E-02  1.3000E-02 1.1021E-15 -1.4318E+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  NI  2.00000E-01  SI  1.30000E-02  CU  2.40000E-03  N   7.00000E-04
 CR  2.46000E-01  MN  1.30000E-02  MO  3.00000E-03  C   9.00000E-04
POLY: 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      0.000000E+00    1.000000E+00
 SUSPENDED PHASES:
 Z_PHASE SIGMA SIC SI3N4 R_PHASE P_PHASE PI NI3TI NBNI3 NB5SI3_D8L MU_PHASE
 MSI2_C40 MSI MP_B31 MOSI2_C11B MO5SI3_D8M MN9SI2 MN6SI MN6N5 MN6N4 MN5SIC
 MN11SI19 MC_SHP MC_ETA M7C3 M6SI5 M6C M5SI3 M5C2 M3SI M3C2 M2P_C22 M23C6
 M11SI8 LAVES_PHASE_C14 KSI_CARBIDE HIGH_SIGMA HCP_A3#2 HCP_A3#1 G_PHASE
 GRAPHITE GAMMA FESI2_L FESI2_H FECN_CHI FE8SI2C FE4N_LP1 FE2SI FCC_A1#2
 DIAMOND_FCC_A4 CUZN_EPSILON CUB_A13 CU6Y CRZN17 CR3SI CHI_A12 CENI5 CENI2
 CEMENTITE CBCC_A12 BETA1 BCC_A2 AL5FE4 AL4C3 LIQUID GAS
 *** STATUS FOR ALL SPECIES
 C        ENTERED    C5       ENTERED    CU2      ENTERED    N2       ENTERED
 C1N1     ENTERED    C5N1     ENTERED    FE       ENTERED    N3       ENTERED
 C1N2_CNN ENTERED    C60      ENTERED    FE+2     ENTERED    NI       ENTERED
 C1N2_NCN ENTERED    C6N1     ENTERED    FE+3     ENTERED    NI+2     ENTERED
 C2       ENTERED    C6N2     ENTERED    FE+4     ENTERED    NI+3     ENTERED
 C2N1_CCN ENTERED    C9N1     ENTERED    MN       ENTERED    SI       ENTERED
 C2N1_CNC ENTERED    CR       ENTERED    MN+2     ENTERED    SI+4     ENTERED
 C2N2     ENTERED    CR+2     ENTERED    MN+3     ENTERED    SI3N4    ENTERED
 C3       ENTERED    CR+3     ENTERED    MN+4     ENTERED    SIN4/3   ENTERED
 C3N1     ENTERED    CU       ENTERED    MO       ENTERED    VA       ENTERED
 C4       ENTERED    CU+1     ENTERED    MO+2     ENTERED
 C4N1     ENTERED    CU+2     ENTERED    N        ENTERED
 C4N2     ENTERED    CU+3     ENTERED    N-3      ENTERED
POLY:Hit RETURN to continue
POLY: s-a-v 1 t
Min value /0/: 200
Max value /1/: 1000
Increment /20/: 10
POLY:
```

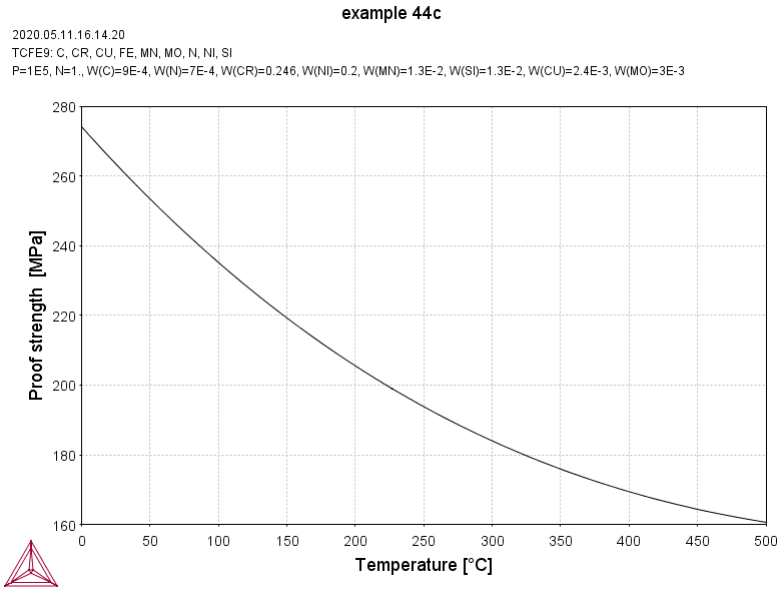
```
POLY: save tcex44 y
POLY: @@ Step in temperature in order to evaluate proof strength
POLY: @@ as a function of temperature.
POLY: step normal
 No initial equilibrium, using default
 Step will start from axis value    500.000
 POLY has calculated initial equilibrium

 Phase Region from    500.000     for:
     FCC_A1#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: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex44\tcex44.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a y rp02
POST: s-d-a x t-c
POST:
POST: set-title example 44a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```




```
POST:
POST:Hit RETURN to continue
POST:
POST: s-s-s x n 0 500
POST:
POST: set-ras y
POST:
POST: set-title example 44b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```



```
POST:
POST:Hit RETURN to continue
POST:
POST: set-axis-text-status
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT  (Y OR N) /N/: n
AXIS TEXT : Proof strength  [MPa]
POST:
POST: set-title example 44c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```




```
POST:
POST: set-inter
POST:
```

tcex48

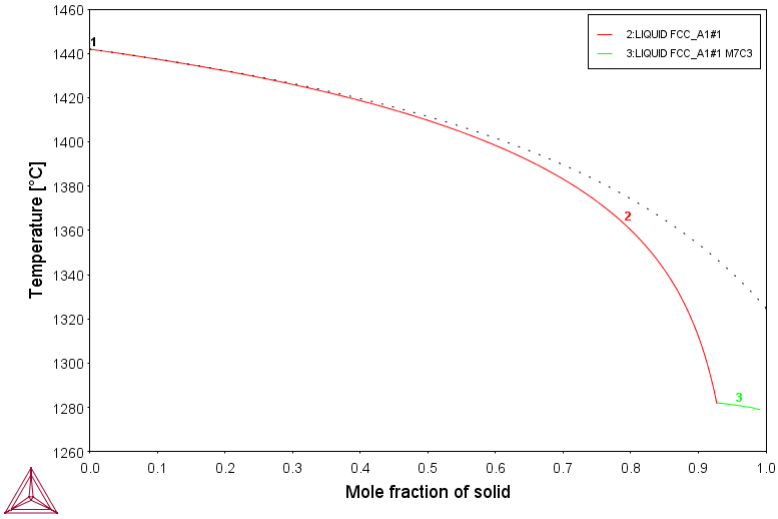
```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex48\tcex48.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Scheil solidification with C back diffusion
SYS:
SYS: @@ This is an example of Scheil solidification with
SYS: @@ C back diffusion in solid phases. The results are
SYS: @@ compared between a simple Scheil and equilibrium
SYS: @@ calculation.
SYS:
SYS: @@ First do ScheiC by assigning C as fast diffuse
SYS: @@ element. Plot solidification and microsegregation
SYS: @@ diagram and save to files
SYS:
SYS: go scheil
SCHEIL: save-file-name tcex48a
SCHEIL: start
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: FEDEMO
 Current database: Iron Demo Database v3.0

 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 GES .....
 FE  DEFINED
 C  DEFINED
 CR  DEFINED


 This database has following phases for the defined system

 GAS:G                    LIQUID:L                 BCC_A2
 LAVES_PHASE_C14          CBCC_A12                 CEMENTITE
 CHI_A12                  CUB_A13                  DIAMOND_FCC_A4
 FCC_A1                   GRAPHITE                 HCP_A3
 KSI_CARBIDE              M23C6                    M3C2
 M5C2                     M7C3                     SIGMA
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

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

    The following phases are retained in this system:

 GAS:G                    LIQUID:L                 BCC_A2
 LAVES_PHASE_C14          CBCC_A12                 CEMENTITE
 CHI_A12                  CUB_A13                  DIAMOND_FCC_A4
 FCC_A1                   GRAPHITE                 HCP_A3
 KSI_CARBIDE              M23C6                    M3C2
 M5C2                     M7C3                     SIGMA

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

OK? /Y/: Y
 GAS:G  REJECTED
16:15:37,416 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
  'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'M. J. Assael, J. Phys. Chem. Ref. Data 35 (2006) 285; Fe, Al'
  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C -Cr-Nb'
  'A.V. Khvan, B. Hallstedt, C. Broeckmann, CALPHAD, 46, 24 -33(2014); Cr-Fe
      -C'
  'P. Gustafson, Scan. J. Metall., 14 (1985) 259-267; TRITA 0237 (1984); C-FE'
  'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
  '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'
  'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
      -CR-FE'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
```

```
  'B.J. Lee, unpublished work at KTH (1999); update of steel database'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
  'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
      TCFE9 database (TCFE v9.0, Jan, 2017).'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'P. Villars, L.D. Calvert. Pearsons handbook of crystallographic data for
      intermetallic phases, Metals park, Ohio 1985: American society for
      metals'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
       CR-FE-MO'
  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992)
      Revision; C-Cr-Fe-Mo'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C -FE-MO'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
      (2011) 479-491; Fe-Mn-C'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
Should any phase have a miscibility gap check? /N/: N
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/: C
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=2273.15, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1    DEGREES OF FREEDOM 0
 PHASE CHANGE AT 1715.05468788
FCC_A1#2 forms
 Testing POLY result by global minimization procedure
Calculated         20164 grid points in             1 s
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

 Phase Region from    1715.14     for:
     LIQUID
 Terminating at    1715.24
 Calculated     4 equilibria

 Phase Region from    1715.14     for:
     LIQUID
 Global check of adding phase at  1.71505E+03
 Calculated     3 equilibria

 Phase Region from    1715.05     for:
     LIQUID
     FCC_A1#1
 Global test at  1.70714E+03 .... OK
 Global test at  1.69714E+03 .... OK
 Global test at  1.68714E+03 .... OK
 Global test at  1.67714E+03 .... OK
 Global test at  1.66714E+03 .... OK
 Global test at  1.65714E+03 .... OK
 Global test at  1.64714E+03 .... OK
 Global test at  1.63714E+03 .... OK
 Global test at  1.62714E+03 .... OK
 Global test at  1.61714E+03 .... OK
 Global test at  1.60714E+03 .... OK
 Global check of removing phase at  1.59813E+03
 Calculated   120 equilibria

 Phase Region from    1598.13     for:
     FCC_A1#1
 Calculated     4 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex48\tcex48a.POLY3
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

 An EXP file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex48\tcex48a_EQ.EXP
 has been created to store the equilibrium solidification results.
  CALCULATING SCHEIL SOLIDFICATION
     T(C)      fraction solid
   1441.995       0.000000
 PHASE REGION:LIQUID + FCC_A1#1
     T(C)      fraction solid
   1441.899      0.1329022E-03
   1440.899      0.2342642E-01
   1439.899      0.4585953E-01
   1438.899      0.6763138E-01
   1437.899      0.8876763E-01
   1436.899      0.1092937
   1435.899      0.1292335
   1434.899      0.1486098
   1433.899      0.1674443
   1432.899      0.1857574
   1431.899      0.2035686
   1430.899      0.2208963
   1429.899      0.2377580
   1428.899      0.2541705
   1427.899      0.2701497
   1426.899      0.2857107
   1425.899      0.3008678
   1424.899      0.3156350
   1423.899      0.3300252
   1422.899      0.3440509
   1421.899      0.3577242
   1420.899      0.3710564
   1419.899      0.3840585
   1418.899      0.3967408
```

1417.899	0.4091133
1416.899	0.4211856
1415.899	0.4329668
1414.899	0.4444657
1413.899	0.4556908
1412.899	0.4666499
1411.899	0.4773509
1410.899	0.4878012
1409.899	0.4980079
1408.899	0.5079779
1407.899	0.5177177
1406.899	0.5272337
1405.899	0.5365319
1404.899	0.5456182
1403.899	0.5544983
1402.899	0.5631775
1401.899	0.5716612
1400.899	0.5799544
1399.899	0.5880619
1398.899	0.5959884
1397.899	0.6037386
1396.899	0.6113168
1395.899	0.6187271
1394.899	0.6259739
1393.899	0.6330609
1392.899	0.6399920
1391.899	0.6467711
1390.899	0.6534016
1389.899	0.6598870
1388.899	0.6662309
1387.899	0.6724363
1386.899	0.6785066
1385.899	0.6844448
1384.899	0.6902539
1383.899	0.6959369
1382.899	0.7014966
1381.899	0.7069357
1380.899	0.7122570
1379.899	0.7174630
1378.899	0.7225564
1377.899	0.7275396
1376.899	0.7324150
1375.899	0.7371850
1374.899	0.7418519
1373.899	0.7464180
1372.899	0.7508854
1371.899	0.7552562
1370.899	0.7595327
1369.899	0.7637168
1368.899	0.7678105
1367.899	0.7718157
1366.899	0.7757345
1365.899	0.7795686
1364.899	0.7833198
1363.899	0.7869901
1362.899	0.7905810
1361.899	0.7940944
1360.899	0.7975319
1359.899	0.8008952
1358.899	0.8041858
1357.899	0.8074053
1356.899	0.8105553
1355.899	0.8136373
1354.899	0.8166528
1353.899	0.8196031
1352.899	0.8224898
1351.899	0.8253143
1350.899	0.8280778
1349.899	0.8307818
1348.899	0.8334275
1347.899	0.8360162
1346.899	0.8385492
1345.899	0.8410277
1344.899	0.8434529
1343.899	0.8458260
1342.899	0.8481482
1341.899	0.8504206
1340.899	0.8526443
1339.899	0.8548203
1338.899	0.8569498
1337.899	0.8590339
1336.899	0.8610734
1335.899	0.8630695
1334.899	0.8650231
1333.899	0.8669352
1332.899	0.8688067
1331.899	0.8706385
1330.899	0.8724315
1329.899	0.8741866
1328.899	0.8759047
1327.899	0.8775867
1326.899	0.8792332
1325.899	0.8808453
1324.899	0.8824235
1323.899	0.8839688
1322.899	0.8854819
1321.899	0.8869634
1320.899	0.8884142
1319.899	0.8898350
1318.899	0.8912264
1317.899	0.8925891
1316.899	0.8939237
1315.899	0.8952310
1314.899	0.8965116
1313.899	0.8977660
1312.899	0.8989948
1311.899	0.9001988
1310.899	0.9013784
1309.899	0.9025342
1308.899	0.9036667
1307.899	0.9047766
1306.899	0.9058642
1305.899	0.9069302
1304.899	0.9079750
1303.899	0.9089992
1302.899	0.9100032

```
  1301.899      0.9109874
  1300.899      0.9119524
  1299.899      0.9128985
  1298.899      0.9138263
  1297.899      0.9147361
  1296.899      0.9156283
  1295.899      0.9165035
  1294.899      0.9173618
  1293.899      0.9182039
  1292.899      0.9190299
  1291.899      0.9198404
  1290.899      0.9206356
  1289.899      0.9214159
  1288.899      0.9221816
  1287.899      0.9229331
  1286.899      0.9236708
  1285.899      0.9243949
  1284.899      0.9251057
  1283.899      0.9258036
  1282.899      0.9264888
  1282.038      0.9271048
PHASE REGION:LIQUID + FCC_A1#1 + M7C3
    T(C)      fraction solid
  1282.007      0.9294370
  1281.007      0.9559107
  1280.007      0.9776564
  1279.007      0.9907091
  1278.007      0.9968826
```

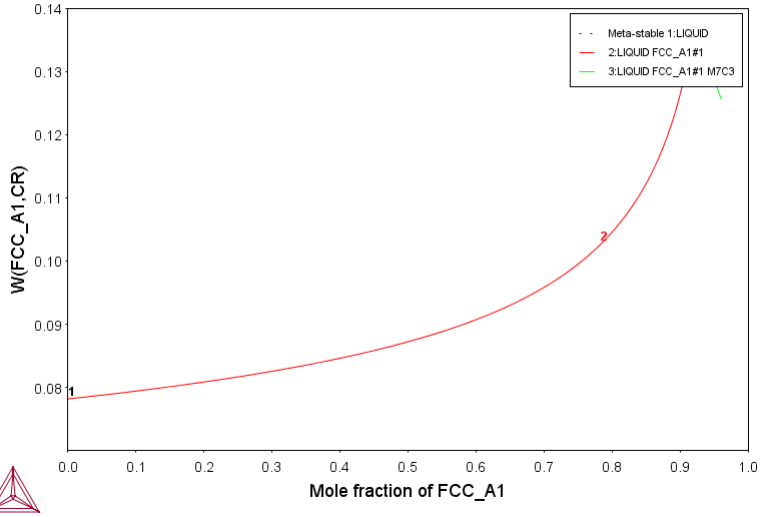
2020.05.11.16.15.44
FEDEMO: C, CR, FE
T=1715.14, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1




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

       The following axis variables are available

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

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

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

```
POST:Hit RETURN to continue
POST: make tcex48a.exp y
POST:
POST: set-dia-ax x ns(fcc_a1)
POST: set-dia-ax y w(fcc_a1,cr)
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,,,,
```

2020.05.11.16.16.07
FEDEMO: C, CR, FE
T=1715.14, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1




```
POST:Hit RETURN to continue
POST:
POST:
POST: make tcex48b.exp y
POST:
POST: back
SCHEIL:
SCHEIL: @@ Ignore back diffusion of C in solids and do Scheil
SCHEIL: @@ with the same alloy by choosing option 3 from the
SCHEIL: @@ Scheil simulation option list.
SCHEIL: @@ Also plot solidification and microsegregation
SCHEIL: @@ diagrams and save to files
SCHEIL:
SCHEIL: save-file-name tcex48b
SCHEIL: start
Database /TCFE10/: FEDEMO
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 1
2nd alloying element: cr 10
Next alloying element:
Temperature (C) /2000/: 1700
 VA                        /-  DEFINED
 REINITIATING GES .....
 FE  DEFINED
 C  DEFINED
 CR  DEFINED


 This database has following phases for the defined system

 GAS:G                     LIQUID:L                  BCC_A2
 LAVES_PHASE_C14           CBCC_A12                  CEMENTITE
 CHI_A12                   CUB_A13                   DIAMOND_FCC_A4
 FCC_A1                    GRAPHITE                  HCP_A3
 KSI_CARBIDE               M23C6                     M3C2
 M5C2                      M7C3                      SIGMA
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

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

    The following phases are retained in this system:

 GAS:G                     LIQUID:L                  BCC_A2
 LAVES_PHASE_C14           CBCC_A12                  CEMENTITE
 CHI_A12                   CUB_A13                   DIAMOND_FCC_A4
 FCC_A1                    GRAPHITE                  HCP_A3
 KSI_CARBIDE               M23C6                     M3C2
 M5C2                      M7C3                      SIGMA

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

OK? /Y/: Y
 GAS:G  REJECTED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 Creating a new composition set FCC_A1#2
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121 -127; Molar
      volumes'
  'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
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  'A.V. Khvan, B. Hallstedt, K. Chang, CALPHAD, 39, 54-61(2012); C -Cr-Nb'
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      -C'
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  'B.J. Lee, CALPHAD, 17 (1993) 251-268; revision of Fe-Cr and Fe -Ni liquid'
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  'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
  'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C
```

```
      -CR-FE'
  'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270
      (1986); CR-FE'
  'N. Saunders, COST 507 Report (1998); Cr-Ti'
  'B.J. Lee, unpublished work at KTH (1999); update of steel database'
  'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equilib., 19
      (1998) 441-448; Fe-Ti'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2019; Cr-Fe-Nb'
  'B.J. Lee, Metall. Trans. A, 24A (1993) 1017-1025; Fe-Cr-Mn-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, Volume data updated for
      TCFE9 database (TCFE v9.0, Jan, 2017).'
  'W. Huang, Metall. Trans. A, 21A (1990) 2115-2123; TRITA-MAC 411 (Rev
      1989); C-FE-MN'
  'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
  'P. Villars, L.D. Calvert. Pearsons handbook of crystallographic data for
      intermetallic phases, Metals park, Ohio 1985: American society for
      metals'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129 -33(2010); Fe-C'
  'P. Gustafson, TRITA-MAC 354 (1987); C-Cr-Fe-Mo-W'
  'J-O. Andersson, Metall. Trans. A, 19A (1988) 1385-1394; TRITA 0322 (1986);
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  'J. Bratberg, Z. Metallkd., 96 (2005) 335-344; Fe-Cr-Mo-C'
  'R. Naraghi, Thermo-Calc Software AB, Sweden, 2016; FCC Fe-Cr-C and C-Cr-Ni'
  'C. Qui, ISIJ International, 32 (1992), 1117-1127; Trita-MAC 482 (1992)
      Revision; C-Cr-Fe-Mo'
  'J-O. Andersson, CALPHAD, 12 (1988) 9-23; TRITA 0321 (1986); C -FE-MO'
  'P. Gustafson, Metall. Trans. A, 19A (1988) 2547-2554; TRITA-MAC 348,
      (1987); C-CR-FE-W'
  'K. Frisk, Metall. Trans. A, 21A (1990) 2477-2488; TRITA 0409 (1989); CR
      -FE-N'
  'D. Djurovic, B. Hallstedt, J. von Appen, R. Dronskowski, Calphad 35.4
      (2011) 479-491; Fe-Mn-C'
  'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
      Sigma model'
 -OK-
Should any phase have a miscibility gap check? /N/: N
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/: NONE
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=1973.15, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1    DEGREES OF FREEDOM 0
 PHASE CHANGE AT 1715.05468788
FCC_A1#1 forms
 Testing POLY result by global minimization procedure
Calculated         20164 grid points in             0 s
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

 Phase Region from    1715.14     for:
     LIQUID
 Terminating at    1715.24
 Calculated     4 equilibria

 Phase Region from    1715.14     for:
     LIQUID
 Global check of adding phase at  1.71505E+03
 Calculated     3 equilibria

 Phase Region from    1715.05     for:
     LIQUID
     FCC_A1#2
 Global test at  1.70714E+03 .... OK
 Global test at  1.69714E+03 .... OK
 Global test at  1.68714E+03 .... OK
 Global test at  1.67714E+03 .... OK
 Global test at  1.66714E+03 .... OK
 Global test at  1.65714E+03 .... OK
 Global test at  1.64714E+03 .... OK
 Global test at  1.63714E+03 .... OK
 Global test at  1.62714E+03 .... OK
 Global test at  1.61714E+03 .... OK
 Global test at  1.60714E+03 .... OK
 Global check of removing phase at  1.59813E+03
 Calculated   120 equilibria

 Phase Region from    1598.13     for:
     FCC_A1#2
 Calculated     4 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex48\tcex48b.POLY3
  POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

 An EXP file c:\jenkins\WORKSP~1\THC20D~1\examples\tcex48\tcex48b_EQ.EXP
 has been created to store the equilibrium solidification results.
  CALCULATING SCHEIL SOLIDFICATION
     T(C)      fraction solid
   1441.995       0.000000
 PHASE REGION:LIQUID + FCC_A1#1
     T(C)      fraction solid
   1441.899      0.1329022E-03
   1440.899      0.2342642E-01
   1439.899      0.4585862E-01
   1438.899      0.6747197E-01
   1437.899      0.8830633E-01
   1436.899      0.1083992
   1435.899      0.1277857
   1434.899      0.1464991
   1433.899      0.1645706
   1432.899      0.1820295
   1431.899      0.1989037
   1430.899      0.2152193
   1429.899      0.2310011
   1428.899      0.2462723
   1427.899      0.2610552
   1426.899      0.2753706
   1425.899      0.2892383
   1424.899      0.3026771
   1423.899      0.3157047
   1422.899      0.3283380
   1421.899      0.3405930
   1420.899      0.3524849
   1419.899      0.3640280
   1418.899      0.3752362
```
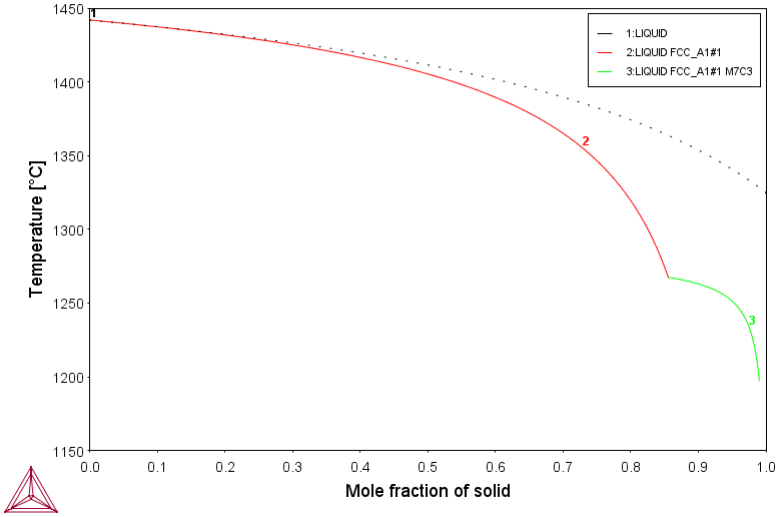

1417.899	0.3861225
1416.899	0.3966992
1415.899	0.4069781
1414.899	0.4169706
1413.899	0.4266874
1412.899	0.4361386
1411.899	0.4453340
1410.899	0.4542829
1409.899	0.4629942
1408.899	0.4714763
1407.899	0.4797374
1406.899	0.4877852
1405.899	0.4956271
1404.899	0.5032702
1403.899	0.5107212
1402.899	0.5179866
1401.899	0.5250727
1400.899	0.5319853
1399.899	0.5387303
1398.899	0.5453131
1397.899	0.5517388
1396.899	0.5580126
1395.899	0.5641393
1394.899	0.5701234
1393.899	0.5759695
1392.899	0.5816819
1391.899	0.5872646
1390.899	0.5927217
1389.899	0.5980568
1388.899	0.6032737
1387.899	0.6083758
1386.899	0.6133667
1385.899	0.6182494
1384.899	0.6230272
1383.899	0.6277031
1382.899	0.6322800
1381.899	0.6367608
1380.899	0.6411480
1379.899	0.6454444
1378.899	0.6496525
1377.899	0.6537746
1376.899	0.6578132
1375.899	0.6617705
1374.899	0.6656487
1373.899	0.6694499
1372.899	0.6731762
1371.899	0.6768295
1370.899	0.6804118
1369.899	0.6839248
1368.899	0.6873704
1367.899	0.6907503
1366.899	0.6940662
1365.899	0.6973196
1364.899	0.7005122
1363.899	0.7036455
1362.899	0.7067209
1361.899	0.7097399
1360.899	0.7127038
1359.899	0.7156140
1358.899	0.7184717
1357.899	0.7212783
1356.899	0.7240349
1355.899	0.7267427
1354.899	0.7294029
1353.899	0.7320165
1352.899	0.7345847
1351.899	0.7371085
1350.899	0.7395889
1349.899	0.7420270
1348.899	0.7444235
1347.899	0.7467796
1346.899	0.7490960
1345.899	0.7513737
1344.899	0.7536136
1343.899	0.7558163
1342.899	0.7579829
1341.899	0.7601140
1340.899	0.7622104
1339.899	0.7642728
1338.899	0.7663021
1337.899	0.7682988
1336.899	0.7702636
1335.899	0.7721973
1334.899	0.7741005
1333.899	0.7759738
1332.899	0.7778178
1331.899	0.7796331
1330.899	0.7814204
1329.899	0.7831801
1328.899	0.7849129
1327.899	0.7866192
1326.899	0.7882996
1325.899	0.7899547
1324.899	0.7915848
1323.899	0.7931906
1322.899	0.7947724
1321.899	0.7963308
1320.899	0.7978662
1319.899	0.7993790
1318.899	0.8008697
1317.899	0.8023387
1316.899	0.8037865
1315.899	0.8052133
1314.899	0.8066196
1313.899	0.8080059
1312.899	0.8093723
1311.899	0.8107195
1310.899	0.8120476
1309.899	0.8133570
1308.899	0.8146482
1307.899	0.8159213
1306.899	0.8171768
1305.899	0.8184150
1304.899	0.8196361
1303.899	0.8208405
1302.899	0.8220285

1301.899	0.8232004
1300.899	0.8243564
1299.899	0.8254969
1298.899	0.8266221
1297.899	0.8277323
1296.899	0.8288277
1295.899	0.8299086
1294.899	0.8309753
1293.899	0.8320279
1292.899	0.8330668
1291.899	0.8340922
1290.899	0.8351043
1289.899	0.8361033
1288.899	0.8370895
1287.899	0.8380631
1286.899	0.8390242
1285.899	0.8399732
1284.899	0.8409101
1283.899	0.8418353
1282.899	0.8427488
1281.899	0.8436510
1280.899	0.8445419
1279.899	0.8454218
1278.899	0.8462908
1277.899	0.8471492
1276.899	0.8479970
1275.899	0.8488346
1274.899	0.8496620
1273.899	0.8504794
1272.899	0.8512869
1271.899	0.8520848
1270.899	0.8528732
1269.899	0.8536522
1268.899	0.8544220
1267.899	0.8551827
1267.548	0.8554471

PHASE REGION:LIQUID + FCC_A1#1 + M7C3

T(C)	fraction solid
1267.517	0.8556564
1266.517	0.8680204
1265.517	0.8787644
1264.517	0.8881677
1263.517	0.8964509
1262.517	0.9037902
1261.517	0.9103282
1260.517	0.9161808
1259.517	0.9214436
1258.517	0.9261957
1257.517	0.9305032
1256.517	0.9344216
1255.517	0.9379979
1254.517	0.9412721
1253.517	0.9442785
1252.517	0.9470463
1251.517	0.9496011
1250.517	0.9519649
1249.517	0.9541568
1248.517	0.9561939
1247.517	0.9580907
1246.517	0.9598604
1245.517	0.9615144
1244.517	0.9630630
1243.517	0.9645153
1242.517	0.9658794
1241.517	0.9671625
1240.517	0.9683712
1239.517	0.9695113
1238.517	0.9705881
1237.517	0.9716065
1236.517	0.9725706
1235.517	0.9734845
1234.517	0.9743516
1233.517	0.9751754
1232.517	0.9759587
1231.517	0.9767042
1230.517	0.9774144
1229.517	0.9780917
1228.517	0.9787380
1227.517	0.9793554
1226.517	0.9799457
1225.517	0.9805103
1224.517	0.9810510
1223.517	0.9815690
1222.517	0.9820657
1221.517	0.9825423
1220.517	0.9829999
1219.517	0.9834395
1218.517	0.9838622
1217.517	0.9842688
1216.517	0.9846601
1215.517	0.9850370
1214.517	0.9854002
1213.517	0.9857504
1212.517	0.9860882
1211.517	0.9864142
1210.517	0.9867291
1209.517	0.9870333
1208.517	0.9873273
1207.517	0.9876116
1206.517	0.9878867
1205.517	0.9881530
1204.517	0.9884108
1203.517	0.9886606
1202.517	0.9889027
1201.517	0.9891375
1200.517	0.9893652
1199.517	0.9895861
1198.517	0.9898005
1197.517	0.9900088
1196.517	0.9902111

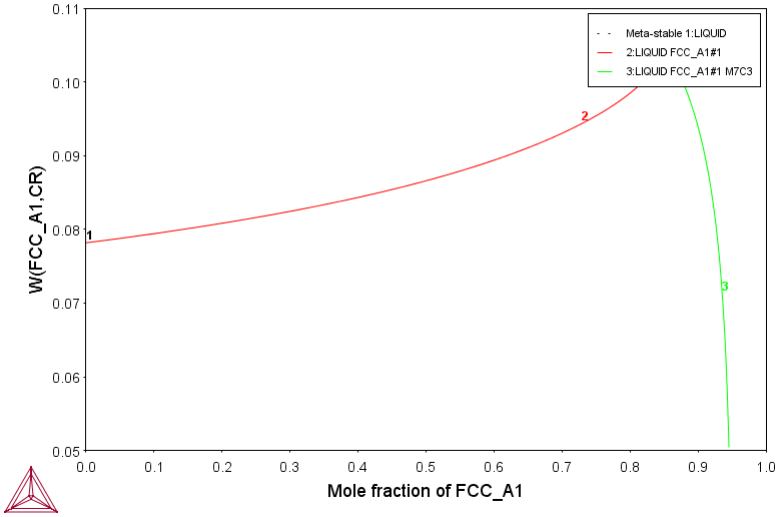
2020.05.11.16.16.11
FEDEMO: C, CR, FE
T=1715.14, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1




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

        The following axis variables are available

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

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

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

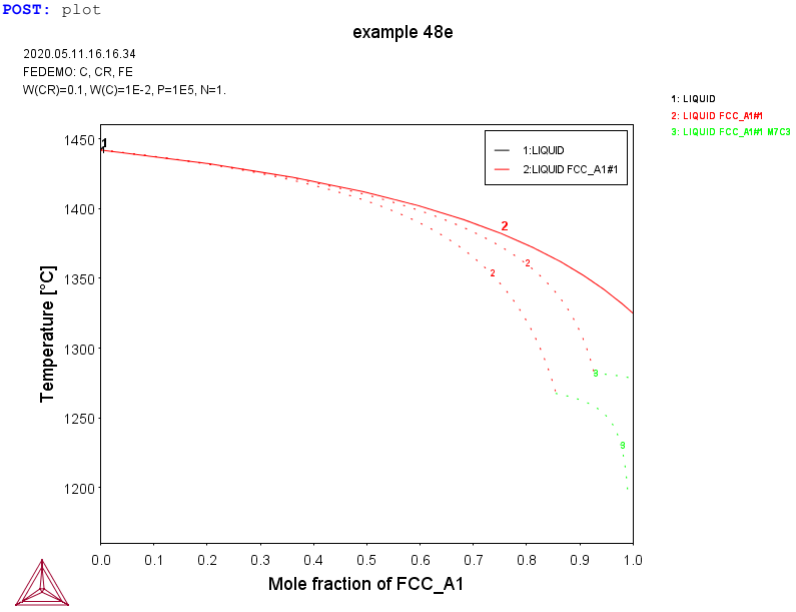
```
POST:Hit RETURN to continue
POST: make tcex48c.exp y
POST: set-dia-ax x ns(fcc_a1)
POST: set-dia-ax y w(fcc_a1,cr)
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot,,,,,
```

2020.05.11.16.16.34
FEDEMO: C, CR, FE
T=1715.14, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1



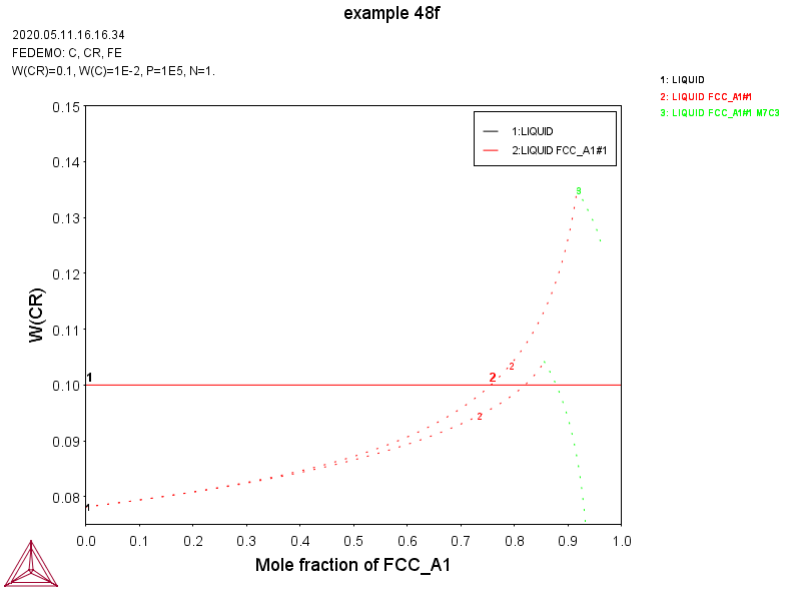

```
POST: make tcex48d.exp y
POST: back
SCHEIL:Hit RETURN to continue
SCHEIL: @@ Calculate simple equilibrium solidification of the
SCHEIL: @@ same alloy and compare the results with those of
SCHEIL: @@ Scheil and ScheiC
SCHEIL: go p-3
POLY: read tcex48b
POLY: list-condition
 T=1715.14, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1
 DEGREES OF FREEDOM 0
POLY: list-equilibrium
OUTPUT TO SCREEN OR FILE /SCREEN/:
```

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

 Conditions:
 T=1715.14, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1
 DEGREES OF FREEDOM 0

 Temperature   1715.14 K (  1441.99 C),  Pressure  1.000000E+05
 Number of moles of components  9.99122E-03,  Mass in grams  4.81052E-01
 Total Gibbs energy -9.65033E+02,  Enthalpy  6.38265E+02,  Volume  7.15495E-08

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 C                       1.6806E-03  4.1961E-02 5.7976E-02 -4.0610E+04 SER
 CR                      8.4601E-04  9.1444E-02 2.0084E-04 -1.2140E+05 SER
 FE                      7.4646E-03  8.6660E-01 1.4494E-03 -9.3215E+04 SER

 LIQUID                     Status ENTERED     Driving force  0.0000E+00
 Moles 9.7889E-03, Mass 4.7122E-01, Volume fraction 9.8061E-01  Mass fractions:
 FE  8.67401E-01  CR  9.05599E-02  C   4.20395E-02

 FCC_A1#1                   Status ENTERED     Driving force  0.0000E+00
 Moles 1.3385E-04, Mass 6.9797E-03, Volume fraction 1.3663E-02  Mass fractions:
 FE  9.31553E-01  CR  5.00131E-02  C   1.84336E-02

 M7C3                       Status ENTERED     Driving force  0.0000E+00
 Moles 6.8452E-05, Mass 2.8511E-03, Volume fraction 5.7305E-03  Mass fractions:
 FE  5.74571E-01  CR  3.38917E-01  C   8.65123E-02
POLY:Hit RETURN to continue
POLY:
POLY: reinit
POLY: set-condition t=1717.15 w(cr)=0.1 w(c)=0.01 p=1e5 n=1
POLY: c-e
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
    31 ITS,  CPU TIME USED   0 SECONDS
POLY: set-ax-var 1 t 500 1717.15 10
POLY: advanced
Which option? /STEP_AND_MAP/: break-condition
Break condition: np(liquid)=0
POLY: save tcex48c y
POLY: step normal
 No initial equilibrium, trying to add one                     0
 Step will start from axis value    1717.15

 Phase Region from    1717.15     for:
     LIQUID
 Calculated     4 equilibria

 Phase Region from    1715.05     for:
     LIQUID
     FCC_A1#1
 Calculated    14 equilibria

 Phase Region from    1598.13     for:
     FCC_A1#1
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex48\tcex48c.POLY3
POLY: post
POST: @@ Define a function to get the amount of solids
POST: ent fun fs=1-np(liquid);
POST: @@ Plot a solidification diagram
POST: set-dia-ax x fs
POST: set-dia-ax y t-c
POST: append-exp y tcex48a tcex48c 0; 1; 0; 1;
POST: set-ax-text x n
AXIS TEXT : Mole fraction of FCC_A1
POST: set-scaling-status y n 1160 1460
POST: set-title example 48e
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```




```
POST:
POST:Hit RETURN to continue
POST:
POST: @@ Plot microsegregation, which represents the composition
POST: @@ profile of the solid. For equilibrium solidification
POST: @@ there is no solute segregation and the composition of
POST: @@ solidified solid is uniform.
```

```
POST:
POST: set-dia-ax x fs
POST: set-dia-ax y w(cr)
POST: append-exp y tcex48b tcex48d 0; 1; 0; 1;
POST: set-ax-text x n
AXIS TEXT : Mole fraction of FCC_A1
POST: set-scaling y n 0.075 0.15
POST: set-title example 48f
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```




```
POST:
POST: set-inter
POST:
```

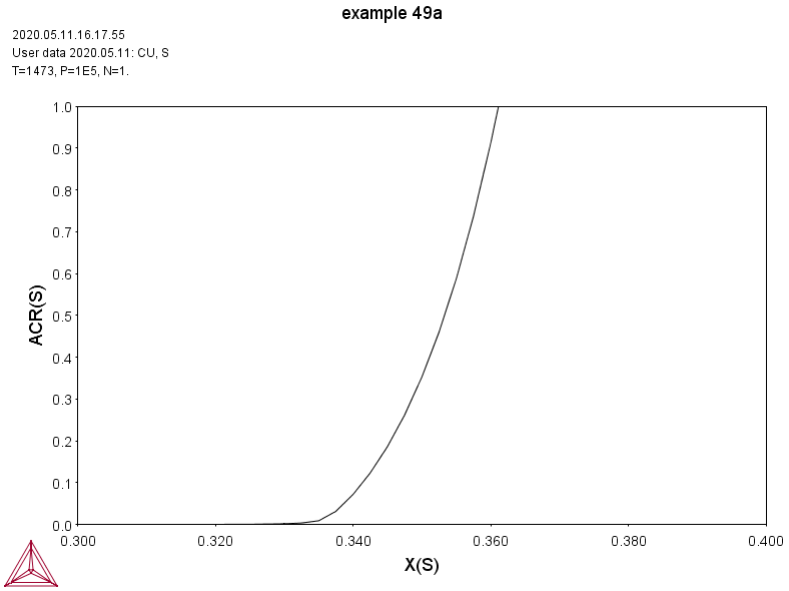
tcex49

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex49\tcex49.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Quasichemical model using the GES module
SYS:
SYS: @@ This example shows how to enter parameters
SYS: @@ for a FACT quasichemical liquid model and
SYS: @@ how to calculate the sulfur activity using
SYS: @@ the Gibbs energy system (GES) module commands.
SYS:
SYS: @@ This example uses some GES commands that are not yet
SYS: @@ supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: set-log ex49,,,
SYS:
SYS: go gibbs
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
GES: ent-el  /- VA CU S
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 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
GES: @@ 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
GES: @@ 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
```

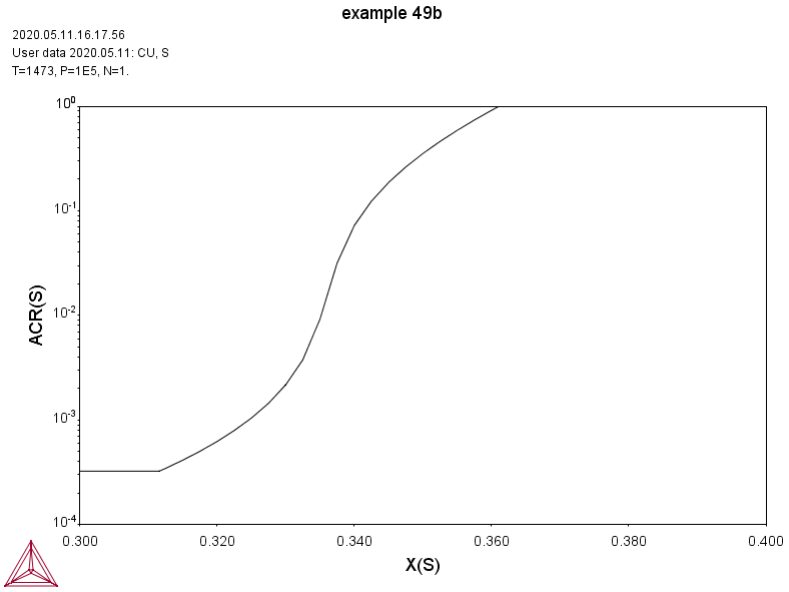
```
& -.00101380333*T**3;  4.53150E+02  Y
FUNCTION: +92539.872-1336.36627*T+202.958*T*LN(T)-.2531915*T**2
& +5.18835E-05*T**3-8202200*T**(-1);  7.17000E+02  Y
FUNCTION: -6889.972+176.35482*T-32*T*LN(T);  1.30000E+03  N
GES: ent-sym fun GCULIQ    2.98150E+02  +12964.84-9.510243*T
   ... the command in 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
GES: @@ to FACT quasichemical model
GES:
GES: amend-phase-description QUASI quasi-fact00
GES:
GES: @@ Binary excess Legendre with 1 as independent
GES: @@ Note that the order of the species are important.
GES:
GES: amend-phase-description QUASI excess
MODEL NAME /REDLICH-KISTER_MUGGIANU/: mixed
First (the independent) constituent: CUQ
Second (the dependent) constituent: CUQS
Excess model type: /LEGENDRE/: Legendre
```

```
 Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent: NONE
GES:
GES:
GES:
GES: list-data
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

 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
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)
 103 GQCU      20000000 +16547-7.6815*T
 104 GQS       20000000 -65357+165.396*T-13.513*T*LN(T)
 105 GHSERCU   20000000
       298.15<T< 1358.02: -7770.458+130.485403*T-24.112392*T*LN(T)
     -.00265684*T**2+1.29223E-07*T**3+52478*T**(-1)
      1358.02<T< 3200.00: -13542.33+183.804197*T-31.38*T*LN(T)
     +3.64643E+29*T**(-9)
 106 GS2GAS    20000000
       298.15<T< 1000.00: +117374.548+2.98629558*T-34.09678*T*LN(T)
     -.002325464*T**2+1.85480167E-07*T**3+128593.6*T**(-1)
      1000.00<T< 3400.00: +117352.438+2.50383258*T-34.04744*T*LN(T)
     -.0021150245*T**2+9.16602333E-08*T**3+175718.45*T**(-1)
      3400.00<T< 6000.00: +124361.091+14.5182895*T-36.1923*T*LN(T)
     -5.930925E-04*T**2-7.54259333E-09*T**3-7484105*T**(-1)
 107 GSSLIQ    20000000
       298.15<T<  388.36: -4001.549+77.889686*T-15.504*T*LN(T)-.018629*T**2
     -2.4942E-07*T**3-113945*T**(-1)
       388.36<T<  428.15: -5285183.35+118449.585*T-19762.4*T*LN(T)
     +32.79275*T**2-.0102214167*T**3+2.646735E+08*T**(-1)
       428.15<T<  432.25: -8174995.23+319914.078*T-57607.3*T*LN(T)
     +135.3045*T**2-.0529973333*T**3
       432.25<T<  453.15: -219408.801+7758.83993*T-1371.85*T*LN(T)
     +2.845035*T**2-.00101380333*T**3
       453.15<T<  717.00: +92539.872-1336.36627*T+202.958*T*LN(T)
     -.2531915*T**2+5.18835E-05*T**3-8202200*T**(-1)
       717.00<T< 1300.00: -6889.972+176.35482*T-32*T*LN(T)
 108 GCULIQ    20000000
       298.15<T< 1358.02: +12964.84-9.510243*T-5.83932E-21*T**7+GHSERCU
      1358.02<T< 3200.00: +13495.4-9.920463*T-3.64643E+29*T**(-9)+GHSERCU


GES:
GES:Hit RETURN to continue
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:

POLY:
```

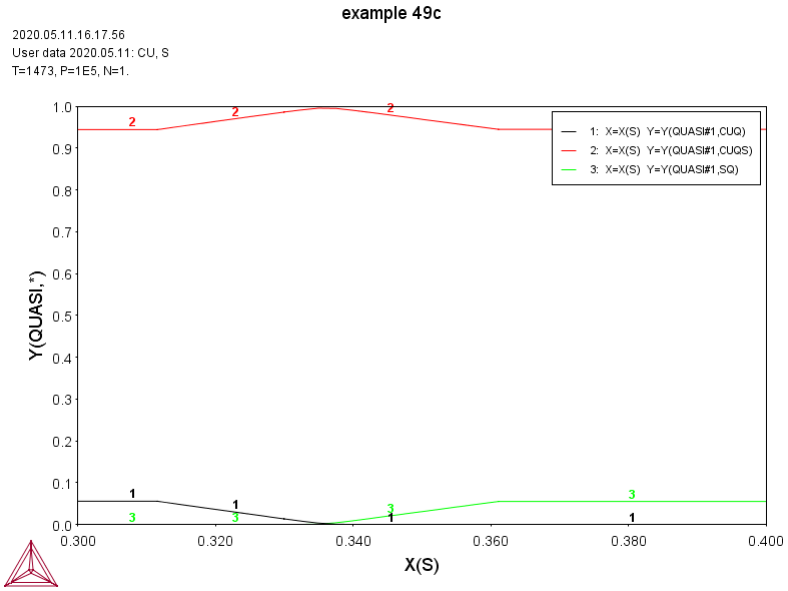
```
POLY:
POLY: l-st ph
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    0.000000E+00
 QUASI                    ENTERED      0.000000E+00    0.000000E+00
 GAS                      ENTERED      0.000000E+00    0.000000E+00
POLY: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY: c-st p q gas
   ... the command in full is CHANGE_STATUS
Status: /ENTERED/: ENTERED
Start value, number of mole formula units /0/: 0
POLY:
POLY:
POLY: s-c t=1473 p=1e5 n=1 x(s)=.33
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1966 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: l-e
   ... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=1473, P=1E5, N=1, X(S)=0.33
 DEGREES OF FREEDOM 0

 Temperature   1473.00 K (  1199.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.31576E+01
 Total Gibbs energy -1.24169E+05,  Enthalpy  1.52783E+04,  Volume  0.00000E+00

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 CU                      6.7000E-01  8.0094E-01 8.2231E-04 -8.6997E+04 SER
 S                       3.3000E-01  1.9906E-01 8.3318E-08 -1.9964E+05 SER

 QUASI                       Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 5.3158E+01, Volume fraction 0.0000E+00  Mass fractions:
 CU  8.00936E-01  S   1.99064E-01
POLY:Hit RETURN to continue
POLY: s-r-s s gas
   ... the command in full is SET_REFERENCE_STATE
Temperature /*/: *
Pressure /1E5/: 1E5
POLY: sh acr(s)
   ... the command in full is SHOW_VALUE
 ACR(S)=2.1652884E-3
POLY:Hit RETURN to continue
POLY: 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: save tcex49 y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.330000
...OK

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.61133E-01
 Calculated    15 equilibria

 Phase Region from   0.361133     for:
     GAS
     QUASI
 Global test at  3.80000E-01 .... OK
 Terminating at   0.400000
 Calculated    19 equilibria

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.10000E-01 .. Creating a new composition set QUASI#2
 Backtracking to find phase change for QUASI#2
 Global test at  3.27500E-01 .... OK
 Global test at  3.22500E-01 .... OK
 Global test at  3.17500E-01 .... OK
 Global test at  3.12500E-01 .... OK
 Global check of adding phase at  3.11581E-01
 Calculated    11 equilibria

 Phase Region from   0.311581     for:
     QUASI#1
     QUASI#2
 Terminating at   0.300000
 Calculated     8 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex49\tcex49.POLY3
POLY: po
   ... the command in full is POST
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y acr(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49a
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: s-a-ty y log
   ... the command in full is SET_AXIS_TYPE
POST: set-title example 49b
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

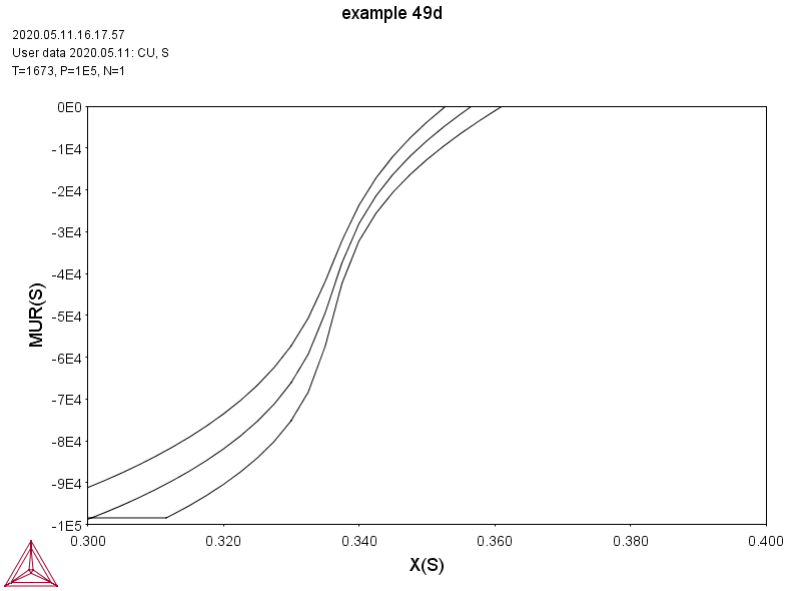



```
POST:
POST:Hit RETURN to continue
POST: s-d-a y y(quasi,*)
   ... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: s-a-ty y lin
   ... the command in full is SET_AXIS_TYPE
POST: s-lab d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 49c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:
POST:@?
POST: back
POLY: read tcex49
   ... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: s-c t=1573
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1966 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: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.330000
...OK

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.56605E-01
 Calculated    13 equilibria

 Phase Region from   0.356605     for:
     GAS
     QUASI
 Global test at  3.75000E-01 .... OK
 Global test at  4.00000E-01 .... OK
 Terminating at   0.400000
 Calculated    21 equilibria

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.10000E-01 .... OK
 Terminating at   0.300000
 Calculated    15 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex49\tcex49.POLY3
POLY:
POLY: read tcex49
   ... the command in full is READ_WORKSPACES
POLY:
POLY:
POLY: s-c t=1673
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1966 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: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value   0.330000
...OK

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.50000E-01 .... OK
 Global check of adding phase at  3.52789E-01
 Calculated    12 equilibria

 Phase Region from   0.352789     for:
     GAS
     QUASI
 Global test at  3.72500E-01 .... OK
 Global test at  3.97500E-01 .... OK
 Terminating at   0.400000
 Calculated    22 equilibria

 Phase Region from   0.330000     for:
     QUASI
 Global test at  3.10000E-01 .... OK
 Terminating at   0.300000
 Calculated    15 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex49\tcex49.POLY3
POLY:
```

```
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: s-d-a y mur(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x x(s)
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49d
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
 Creating a new composition set QUASI#2
 The composition set QUASI#2 created from the store file
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex51

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

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 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex51\tcex51.TCM.test"
SYS: set-echo
SYS:
SYS: @@ Calculation of molar volume,
SYS: @@ thermal expansivity and density.
SYS:
SYS: @@ This example uses the POLY3 module to calculate
SYS: @@ the molar volume, thermal expansivity and density
SYS: @@ of the FCC_A1, BCC_A2 LIQUID and liquid phases of C-Fe.
SYS:
SYS: @@ Note that a TCFE database license is required to run
SYS: @@ the example.
SYS:
SYS: set-log ex51,,
SYS:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw tcfe9
   ... the command in full is SWITCH_DATABASE
 Current database: Steels/Fe-Alloys  v9.2

 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
TDB_TCFE9:
TDB_TCFE9: @@ Volume of a unary system
TDB_TCFE9: d-sys fe
   ... the command in full is DEFINE_SYSTEM
 FE  DEFINED
TDB_TCFE9: rej-ph * all
   ... the command in full is REJECT
 LIQUID:L                BCC_A2                  FCC_A1
 HCP_A3                  CBCC_A12                CUB_A13
 LAVES_PHASE_C14         AL5FE4                  M2O3C:I
   REJECTED
TDB_TCFE9: rest-ph fcc_a1,bcc_a2,liquid
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  LIQUID:L
   RESTORED
TDB_TCFE9: get
   ... the command in full is GET_DATA
16:19:14,773 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 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, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
 -OK-
TDB_TCFE9:
TDB_TCFE9: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: s-c t=400, n=1, p=1e5
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated             3 grid points in             2 s
POLY: s-a-v 1 t 298 2000,,
   ... the command in full is SET_AXIS_VARIABLE
POLY:

POLY: save tcex51 y
   ... the command in full is SAVE_WORKSPACES
POLY: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    400.000
...OK

 Phase Region from    400.000     for:
     BCC_A2
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global test at  1.08000E+03 .... OK
 Global test at  1.18000E+03 .... OK
```
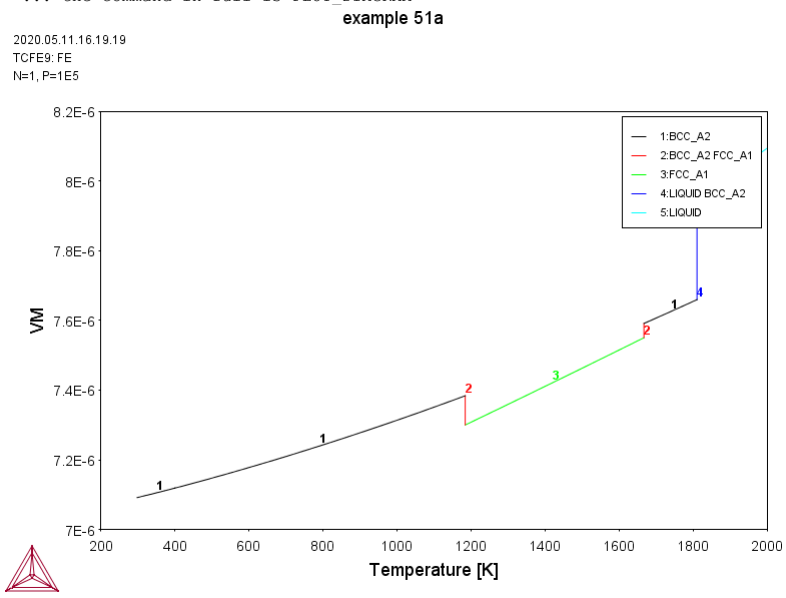
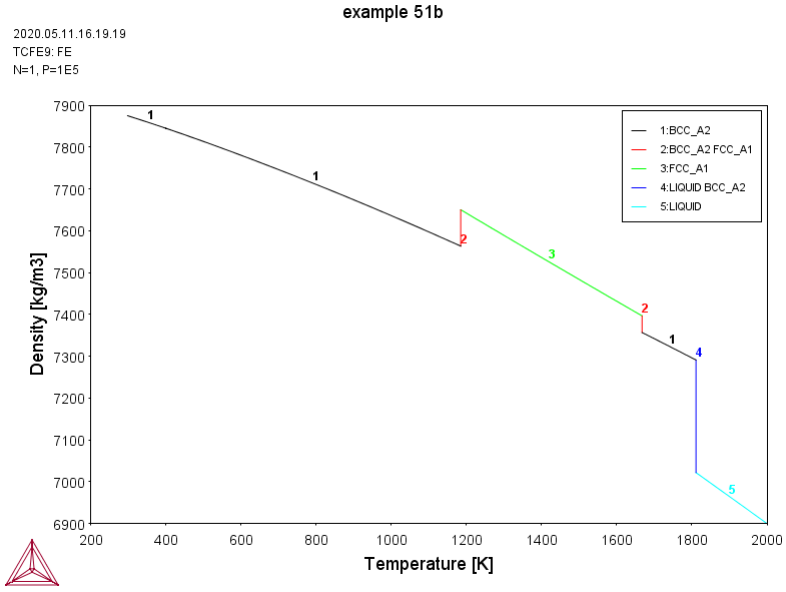

```
 Global check of adding phase at  1.18481E+03
 Calculated    81 equilibria

 Phase Region from    1184.81     for:
     BCC_A2
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    1184.81     for:
     FCC_A1
 Global test at  1.26000E+03 .... OK
 Global test at  1.36000E+03 .... OK
 Global test at  1.46000E+03 .... OK
 Global test at  1.56000E+03 .... OK
 Global test at  1.66000E+03 .... OK
 Global check of adding phase at  1.66747E+03
 Calculated    51 equilibria

 Phase Region from    1667.47     for:
     BCC_A2
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    1667.47     for:
     BCC_A2
 Global test at  1.74000E+03 .... OK
 Global check of adding phase at  1.81095E+03
 Calculated    18 equilibria

 Phase Region from    1810.95     for:
     LIQUID
     BCC_A2
 Calculated     2 equilibria

 Phase Region from    1810.95     for:
     LIQUID
 Global test at  1.89000E+03 .... OK
 Global test at  1.99000E+03 .... OK
 Terminating at    2000.00
 Calculated    22 equilibria

 Phase Region from    400.000     for:
     BCC_A2
 Global test at  3.20000E+02 .... OK
 Terminating at    298.000
 Calculated    14 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex51\tcex51.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51a
POST: s-l e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```

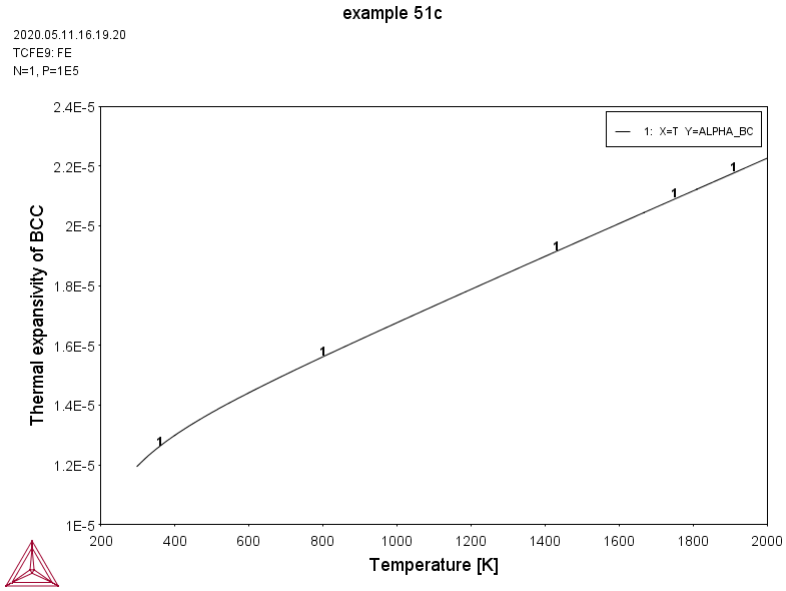



```
POST:
POST:Hit RETURN to continue
POST: @@ Define and plot density
POST: ent fun density=b*1e-3/vm;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y density
   ... the command in full is SET_DIAGRAM_AXIS
POST: set-axis-text y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Density [kg/m3]
POST: set-title example 51b
POST:
POST:
```

```
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```



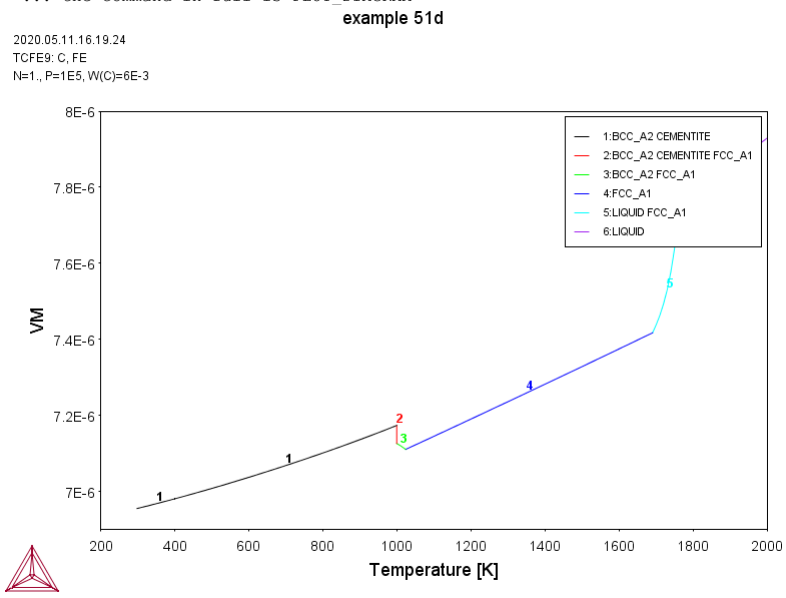

```
POST:
POST:Hit RETURN to continue
POST: @@ Define and plot coefficient of linear
POST: @@ thermal expansion
POST: ent fun alpha_bcc_a2=vm(bcc_a2).t/vm(bcc_a2)/3;
   ... the command in full is ENTER_SYMBOL
POST: s-d-a y alpha_bcc_a2
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
   ... the command in full is SET_LABEL_CURVE_OPTION
POST: set-axis-text y n
   ... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Thermal expansivity of BCC
POST: set-title example 51c
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST:Hit RETURN to continue
POST: back
POLY: @@ Volume of Fe-C binary system
POLY: go da
   ... the command in full is GOTO_MODULE
TDB_TCFE9: rej sys
   ... the command in full is REJECT
 VA                      /-  DEFINED
 L12_FCC                 B2_BCC                  DICTRA_FCC_A1
   REJECTED
 REINITIATING GES .....
TDB_TCFE9: de-sys fe c
   ... the command in full is DEFINE_SYSTEM
 FE                      C  DEFINED
TDB_TCFE9: rej-ph * all
   ... the command in full is REJECT
 GAS:G                   LIQUID:L                BCC_A2
```

```
 FCC_A1                  HCP_A3                  CBCC_A12
 CUB_A13                 DIAMOND_FCC_A4          GRAPHITE
 CEMENTITE               M23C6                   M7C3
 M5C2                    KSI_CARBIDE             FE4N_LP1
 FECN_CHI                LAVES_PHASE_C14         AL5FE4
 M2O3C:I  REJECTED
TDB_TCFE9: res-ph fcc_a1,bcc_a2,cementite,liquid
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2                  CEMENTITE
 LIQUID:L  RESTORED
TDB_TCFE9: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'B. Uhrenius, Int. J. Refract. Met. Hard Mater. 12 (1994) 121-127; Molar
      volumes'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar
      volumes'
  '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. Hallstedt, unpublished work (2016); C-Fe-Mn Epsilon martensite.'
  'B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F.
      Koermann, T. Hickel, J. Neugebauer, CALPHAD, 34, 129-33(2010); Fe-C'
 -OK-
TDB_TCFE9:
TDB_TCFE9: go poly
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: s-c t=400, n=1, p=1e5
   ... the command in full is SET_CONDITION
POLY: s-c w(c)=.6e-2
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           628 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: s-a-v 1 t 298 2000,,
   ... the command in full is SET_AXIS_VARIABLE
POLY:
POLY: 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: step normal
   ... the command in full is STEP_WITH_OPTIONS
 No initial equilibrium, using default
 Step will start from axis value    400.000
...OK

 Phase Region from    400.000     for:
     BCC_A2
     CEMENTITE
 Global test at  4.80000E+02 .... OK
 Global test at  5.80000E+02 .... OK
 Global test at  6.80000E+02 .... OK
 Global test at  7.80000E+02 .... OK
 Global test at  8.80000E+02 .... OK
 Global test at  9.80000E+02 .... OK
 Global check of adding phase at  9.99685E+02
 Calculated    62 equilibria

 Phase Region from    999.685     for:
     BCC_A2
     CEMENTITE
     FCC_A1
 Calculated     2 equilibria

 Phase Region from    999.685     for:
     BCC_A2
     FCC_A1
 Global check of removing phase at  1.02363E+03
 Calculated     6 equilibria

 Phase Region from    1023.63     for:
     FCC_A1
 Global test at  1.10000E+03 .... OK
 Global test at  1.20000E+03 .... OK
 Global test at  1.30000E+03 .... OK
 Global test at  1.40000E+03 .... OK
 Global test at  1.50000E+03 .... OK
 Global test at  1.60000E+03 .... OK
 Global check of adding phase at  1.69090E+03
 Calculated    70 equilibria

 Phase Region from    1690.90     for:
     LIQUID
     FCC_A1
 Global check of removing phase at  1.76294E+03
 Calculated    10 equilibria

 Phase Region from    1762.94     for:
     LIQUID
 Global test at  1.84000E+03 .... OK
 Global test at  1.94000E+03 .... OK
 Terminating at    2000.00
 Calculated    27 equilibria
```

```
 Phase Region from    400.000     for:
     BCC_A2
     CEMENTITE
 Global test at  3.20000E+02 .... OK
 Terminating at    298.000
 Calculated    14 equilibria
 *** Buffer saved on file: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex51\tcex51.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: s-d-a x t-k
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
   ... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51d
POST: s-l e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
   ... the command in full is PLOT_DIAGRAM
```




```
POST:
POST: set-inter
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex52

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex52\tcex52.TCM.test"
SYS: set-echo
SYS:
SYS:
SYS: @@ Changing the excess models for interaction
SYS: @@ parameters in a solution phase
SYS:
SYS:
SYS: @@ This example shows how to change the excess models for binary
SYS: @@ and ternary interactions in a solution phase, either through
SYS: @@ direct interactive amendments of phase descriptions within
SYS: @@ the GES module, or enforced by specific type-definitions
SYS: @@ given in a database file retrieved by the TDB module.
SYS: @@ ---------------------------------------------------------------
SYS: @@ For Binary Excess Model: from the default R-K model to
SYS: @@   Mixed-Excess-Model (the phase has to be a substitutional phase)
SYS: @@ ---------------------------------------------------------------
SYS: @@ For Ternary Extrapolation Model: from the default R-K-M model to
SYS: @@ Toop_Kohler model
SYS: @@ ---------------------------------------------------------------
SYS: set-log TCEX52.LOG
Heading: Example showing how to enter a TOOP binary extrapolation model
SYS:
SYS:
SYS: @@ This example modifies the database interactively, which is not
SYS: @@ yet supported by GES6. Therefore, we enforce the use of GES5.
SYS: set-ges-version 5
SYS:
SYS: go gibbs
   ... the command in full is GOTO_MODULE
 GIBBS ENERGY SYSTEM
GES: reinitiate ,,,
Default element reference state symbol index /1/:
GES: ent-el  /- VA A B C
   ... the command in full is ENTER_ELEMENT
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
GES:
GES: am_el_d /-  ELECTRON_GAS           0.0000E+00  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d VA  VACUUM                 0.0000E+00  0.0000E+00  0.0000E+00 1
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d A   UNKNOWN                1.0000E+01  0.0000E+00  0.0000E+00 2
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d B   BETA_RHOMBO_B          1.0811E+01  1.2220E+00  5.9000E+00 2
   ... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d C   GRAPHITE               1.2011E+01  1.0540E+00  5.7400E+00 2
   ... the command in full is AMEND_ELEMENT_DATA
GES:
GES: ent-phase LIQUID  L,  1   A,B,C ;  N N
   ... the command in full is ENTER_PHASE
GES:
GES: ent-param G(LIQUID,A;0) 298.15 0; 6000 N!
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,A;0)-H298(UNKNOWN,A;0)
GES: ent-param G(LIQUID,B;0) 298.15 0; 6000 N!
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0)
GES: ent-param G(LIQUID,C;0) 298.15 0; 6000 N!
   ... the command in full is ENTER_PARAMETER
 G(LIQUID,C;0)-H298(GRAPHITE,C;0)
GES:
GES: ent-param L(LIQUID,A,B;0)  298.15  10000;  6000 N
   ... the command in full is ENTER_PARAMETER
 L(LIQUID,A,B;0)
GES: ent-param L(LIQUID,A,B;1)  298.15 -10000;  6000 N
   ... the command in full is ENTER_PARAMETER
 L(LIQUID,A,B;1)
GES:
GES: list-data ,,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

 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
```

```
 LIQUID
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
    CONSTITUENTS: A,B,C

      G(LIQUID,A;0)-H298(UNKNOWN,A;0) =  0.0
      G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) =  0.0
      G(LIQUID,C;0)-H298(GRAPHITE,C;0) =  0.0
      L(LIQUID,A,B;0) = +10000
      L(LIQUID,A,B;1) = -10000

 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


GES:Hit RETURN to continue
GES:
GES: @@ ========================================================
GES: @@ Step 1: Amending the binary excess model:
GES: @@ ========================================================
GES: @@ The default binary excess model is the Redlich-Kister Model
GES: @@ for all the three associated binary interaction pairs
GES: @@ (A-B, A-C and B-C)in the substitutional LIQUID solution
GES: @@ phase (without sublattice) that consists of three elements
GES: @@ (A, B and C).
GES:
GES: @@ Before changing this default binary excess model for the
GES: @@ ternary LIQUID solution phase, one must have already entered
GES: @@ the G parameters (for standard Gibbs energies of all pure
GES: @@ end-members) and L parameters (for binary R-K excess
GES: @@ interaction energies), as shown here.
GES:
GES: @@ In this particular example, we want to change from the
GES: @@ default R-K binary excess model to the Mixed-Excess-Model
GES: @@ (with three different binary excess models, namely Legendre,
GES: @@ Polynom and Redlich-Kister models, applied to the A-B,
GES: @@ A-C and B-C binaries, respectively), as demonstrated below:
GES:
GES: @@ For the A-B interaction, the Legendre binary excess model
GES: @@ should be used (rather than the default Redlich-Kister
GES: @@ Model), with 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: amend-phase-description liquid
AMEND WHAT /COMPOSITION_SETS/: ?
 You can amend
 EXCESS_MODEL
 MAGNETIC_ORDERING
 DEBYE_HUCKEL
 STATUS_BITS
 NEW_CONSTITUENT
 RENAME_PHASE
 COMPOSITION_SETS
 GLASS_TRANSITION
 DISORDERED_PART
 MAJOR_CONSTITUENT
 ZRO2_TRANSITION
 REMOVE_ADDITIONS
 QUASICHEM_IONIC
 QUASICHEM_FACT00
 QUASICHEM_IRSID
 TERNARY_EXTRAPOLAT
 HKF_ELECTROSTATIC
 DEFAULT_STABLE
 SITE_RATIOS
 FRACTION_LIMITS
 NEVER_DISORDER_PAR
AMEND WHAT /COMPOSITION_SETS/: excess
MODEL NAME /REDLICH-KISTER_MUGGIANU/: ?
 REDLICH-KISTER_MUGGIANU
 REDLICH-KISTER_KOHLER
 FLORY-HUGGINS POLYMER MODEL
 MIXED-EXCESS-MODELS (R-K default)
 HKF
 PITZER
 CENTRAL_ATOM_MODEL

MODEL NAME /REDLICH-KISTER_MUGGIANU/: mixed
First (the independent) constituent: ?
 FILE SYSTEM ERROR IN FILHLP
 ERROR                   1717  READING HELP FILE
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 ,,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

 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


 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C

      G(LIQUID,A;0)-H298(UNKNOWN,A;0) =  0.0
      G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) =  0.0
      G(LIQUID,C;0)-H298(GRAPHITE,C;0) =  0.0
$ Binary excess model Legendre with A as independent
      L(LIQUID,A,B;0) = +10000
      L(LIQUID,A,B;1) = -10000

 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


GES:Hit RETURN to continue
GES:
GES: @@ For the A-C interaction, the Polynom binary excess model
GES: @@ should be used (rather than the default Redlich-Kister
GES: @@ Model), with the second species (i.e. C) as the
GES: @@ independent constituent and the first species (i.e. A)
GES: @@ as the dependent constituent, while the L parameters for
GES: @@ the A-C interaction shall remain the same as those
GES: @@ 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 ,,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

 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



 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C

      G(LIQUID,A;0)-H298(UNKNOWN,A;0) =  0.0
      G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) =  0.0
      G(LIQUID,C;0)-H298(GRAPHITE,C;0) =  0.0
$ Binary excess model Legendre with A as independent
      L(LIQUID,A,B;0) = +10000
      L(LIQUID,A,B;1) = -10000
$ Binary excess model Polynom with C as independent
      L(LIQUID,A,C;0) = +10000
      L(LIQUID,A,C;1) = +5000

 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


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
GES: @@ amend 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 ,,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11

 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


 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C

      G(LIQUID,A;0)-H298(UNKNOWN,A;0) =  0.0
      G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) =  0.0
      G(LIQUID,C;0)-H298(GRAPHITE,C;0) =  0.0
$ Binary excess model Legendre with A as independent
      L(LIQUID,A,B;0) = +10000
      L(LIQUID,A,B;1) = -10000
$ Binary excess model Polynom with C as independent
      L(LIQUID,A,C;0) = +10000
      L(LIQUID,A,C;1) = +5000
      L(LIQUID,B,C;0) = +10000
      L(LIQUID,B,C;1) = -2000

 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


GES:Hit RETURN to continue
GES:
GES: @@ ========================================================
GES: @@ Step 2: Amending the ternary extrapolation model:
GES: @@ ========================================================
GES: @@ The default ternary excess model is the
GES: @@ Redlich-Kister_Muggianu Model (i.e., the MUGGIANU_RESTOR
GES: @@ method for ternary extrapolation based on binary parameters)
GES: @@ for the associated ternary interaction terms; when no
GES: @@ ternary L parameter is entered for that, such a default
GES: @@ Redlich-Kister_Muggianu Model is thus to be used for
GES: @@ extrapolation from binary excess energies to ternary
GES: @@ interactions in the substitutional LIQUID solution phase
GES: @@ (without sublattice) that consists of three elements
GES: @@ (A, B and C).
GES:
GES: @@ However, in this particular example as follows.
GES: @@ We shall change from this default R-K-M ternary excess
GES: @@ model to the TOOP-KOHLER method for the ternary extrapolation
GES: @@ method, with the species C as the Toop constituent, while
GES: @@ the species A and B as the Kohler constituents (entering A
GES: @@ and B, or B and A, as the basis constituent and first
GES: @@ interacting constituent). This implicitly enforces that,
GES: @@ during the ternary extrapolation, only the A-B binary
GES: @@ interaction parameters are utilized in accordance with the
GES: @@ 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)
GES: @@ are used in line with the Toop-Kohler ternary extrapolation
GES: @@ formula (for the A-C-B and B-C-A ternary interactions). This
GES: @@ makes the extrapolated ternary excess interaction terms
GES: @@ different from those handled either by the default
GES: @@ MUGGIANU_RESTOR method or by the alternative KOHLER-ALL
GES: @@ method.
GES:
GES: @@ Note that only when all the relevant binary excess energies
GES: @@ in a ternary system are treated by the default Redlich-Kister
GES: @@ Model (i.e., the Mixed-Excess-Model should have not been
GES: @@ used), the MUGGIANU_RESTOR method for ternary extrapolations
GES: @@ is equivalent to the Redlich-Kister_Muggianu Model, or the
GES: @@ KOHLER-ALL method to the Redlich-Kister_Kohler Model.
GES:
GES: amend_phase-des LIQUID
   ... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION_SETS/: ?
 You can amend
 EXCESS_MODEL
 MAGNETIC_ORDERING
 DEBYE_HUCKEL
 STATUS_BITS
 NEW_CONSTITUENT
 RENAME_PHASE
 COMPOSITION_SETS
 GLASS_TRANSITION
 DISORDERED_PART
 MAJOR_CONSTITUENT
 ZRO2_TRANSITION
 REMOVE_ADDITIONS
 QUASICHEM_IONIC
 QUASICHEM_FACT00
 QUASICHEM_IRSID
 TERNARY_EXTRAPOLAT
 HKF_ELECTROSTATIC
 DEFAULT_STABLE
 SITE_RATIOS
 FRACTION_LIMITS
 NEVER_DISORDER_PAR
AMEND WHAT /COMPOSITION_SETS/: TERN-EXT
Extrapolation method: /TOOP-KOHLER/: ?
 Default method is Muggianu, you can use
 TOOP-KOHLER
 KOHLER-ALL
 MUGGIANU_RESTOR
Extrapolation method: /TOOP-KOHLER/: TOOP-KOHLER
Constituent in sublattice 1: A
First interaction constituent: B
Toop constituent: C
GES:
GES: list-data ,,

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT        DATE 2020- 5-11
 FROM DATABASE: User data 2020.05.11
```

```
 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



 LIQUID
 EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)
    CONSTITUENTS: A,B,C

      G(LIQUID,A;0)-H298(UNKNOWN,A;0) =  0.0
      G(LIQUID,B;0)-H298(BETA_RHOMBO_B,B;0) =  0.0
      G(LIQUID,C;0)-H298(GRAPHITE,C;0) =  0.0
$ Binary excess model Legendre with A as independent
$ Ternary extrapolation for LIQUID using KOHLER           A B C
      L(LIQUID,A,B;0) = +10000
      L(LIQUID,A,B;1) = -10000
$ Binary excess model Polynom with C as independent
$ Ternary extrapolation for LIQUID using TOOP-KOHLER      A C B
      L(LIQUID,A,C;0) = +10000
      L(LIQUID,A,C;1) = +5000
$ Ternary extrapolation for LIQUID using TOOP-KOHLER      B C A
      L(LIQUID,B,C;0) = +10000
      L(LIQUID,B,C;1) = -2000

 SYMBOL        STATUS   VALUE/FUNCTION
 FUNCTION R          298.15    8.31451000000000     ; 6000 N REF0 !
   2 RTLNP     20000000 +R*T*LN(1E-05*P)


GES:Hit RETURN to continue
GES: @@ ==========================================================
GES: @@ Step 3: Performing an equilibrium calculation using the
GES: @@         entered and amended descriptions.
GES: @@ ==========================================================
GES:
GES: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1965 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: l-e , X
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: User dat

 Conditions:
 T=1500, P=1E5, N=1, X(B)=0.2, X(C)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1500.00 K (  1226.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.07655E+01
 Total Gibbs energy -1.08432E+04,  Enthalpy  1.99843E+03,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       5.0000E-01  5.0000E-01 4.7833E-01 -9.1973E+03 SER
 B                       2.0000E-01  2.0000E-01 1.9875E-01 -2.0151E+04 SER
 C                       3.0000E-01  3.0000E-01 5.5332E-01 -7.3811E+03 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0765E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.00000E-01  C  3.00000E-01  B  2.00000E-01
POLY: sh qf(*)
   ... the command in full is SHOW_VALUE
 QF(LIQUID)=0.52168269
POLY: sh gm(*) dgm(*)
   ... the command in full is SHOW_VALUE
 GM(LIQUID)=-10843.162
 DGM(LIQUID)=0
POLY:

POLY: save TCEX52a.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continue
POLY: @@ ==========================================================
POLY: @@ Step 4: Reading the same data from a small database and
POLY: @@         Performing the same equilibrium calculation.
POLY: @@ ==========================================================
POLY:
POLY: go data
   ... the command in full is GOTO_MODULE
TDB_TCFE10: rej sys
   ... the command in full is REJECT
 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
 REINITIATING GES .....
TDB_TCFE10:
TDB_TCFE10: 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 .......
 WARNING: IN TDBEPH, ILLEGAL TYPE-DEFINITION "%"  AT PHASE LIQUID
 PARAMETERS ...
 FUNCTIONS ....
 AFTER ...
   ... the command in full is AMEND_PHASE_DESCRIPTION
 *** ERROR  1413 IN GZXFX : No interaction record, do this AFTER entering parameters
  ERROR                    1413  RESET
   ... the command in full is AMEND_PHASE_DESCRIPTION
 -OK-
TDB_USER:
TDB_USER:Hit RETURN to continue
TDB_USER: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:
POLY: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
   ... the command in full is SET_CONDITION
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1965 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: l-e , X
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1500, P=1E5, N=1, X(B)=0.2, X(C)=0.3
 DEGREES OF FREEDOM 0

 Temperature   1500.00 K (  1226.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  1.07655E+01
 Total Gibbs energy -1.28416E+04,  Enthalpy  0.00000E+00,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 A                       5.0000E-01  5.0000E-01 5.0000E-01 -8.6448E+03 SER
 B                       2.0000E-01  2.0000E-01 2.0000E-01 -2.0073E+04 SER
 C                       3.0000E-01  3.0000E-01 3.0000E-01 -1.5016E+04 SER

 LIQUID                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 1.0766E+01, Volume fraction 0.0000E+00  Mole fractions:
 A  5.00000E-01  C  3.00000E-01  B  2.00000E-01
POLY: sh qf(*)
   ... the command in full is SHOW_VALUE
 QF(LIQUID)=1
POLY: sh gm(*) dgm(*)
   ... the command in full is SHOW_VALUE
 GM(LIQUID)=-12841.59
 DGM(LIQUID)=0
POLY:
POLY: save TCEX52b.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY:
POLY:
POLY: @@ As you have noticed, the calculated equilibrium (using the
POLY: @@ small database) is exactly the same as the first
POLY: @@ calculation (with data amended in the GES module
POLY: @@ step-by-step, for the binary/ternary excess models).
POLY:
POLY:
POLY: set-inter
   ... the command in full is SET_INTERACTIVE
POLY:
```

tcex53

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex53\tcex53.TCM.test"
SYS: go sys
SYS: set-echo
SYS:
SYS: set-log TCEX53.LOG
Heading: Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine
SYS:
SYS: @@ Some Pourbaix diagrams
SYS:
SYS:
SYS: @@ ==========================================================
SYS: @@   Copyright: Thermo-Calc Software AB, Stockholm, Sweden
SYS: @@   Developer: Dr. Pingfang Shi, Thermo-Calc Software AB
SYS: @@   Date:      2014-05-26 (revision)
SYS: @@   Text updated July 2017 (AJW)
SYS:
SYS: @@ ==========================================================
SYS: @@ Example description:
SYS: @@ ==========================================================
SYS: @@ TCEX53 uses the PAQ2 database to calculate some Pourbaix
SYS: @@ diagrams. The DATABASE_RETRIEVAL (TDB),
SYS: @@ GIBBS_ENERGY_SYSTEM (GES), POLY3, and POSTÂ modules are
SYS: @@ used for the Fe-X-H2O-NaCl heterogeneous interaction
SYS: @@ system, where X = Cr-Ni-Co.
SYS:
SYS: @@ Note: The initial bulk composition of Fe-based alloy in
SYS: @@ this calculation is only preliminarily assigned, in which
SYS: @@ the BCC_A2 and/or FCC_A1 solution phase(s) are considered
SYS: @@ as of primarily interest. For practical calculations,
SYS: @@ you need more precise inputs for the initial bulk
SYS: @@ compositions of alloys.
SYS:
SYS: @@ ==========================================================
SYS: @@ Notes about the example and the PAQ2 database:
SYS: @@ ==========================================================
SYS: @@ The so-called Pourbaix diagram is actually a phase diagram
SYS: @@ with independently-varied electropotential (Eh) and
SYS: @@ acidity (pH),for an heterogeneous interaction system at a
SYS: @@ certain bulk composition (that is by default always set as
SYS: @@ 1 kg of water  solving a specified amount of metals and
SYS: @@ other solutes), under defined temperature and pressure
SYS: @@ conditions.
SYS:
SYS: @@ The PAQ2 database is specially designed for Pourbaix
SYS: @@ diagram calculations (i.e., Eh-pH plots). It contains an
SYS: @@ AQUEOUS solution phase and REF_ELECTRODE phase (as a
SYS: @@ reference for electron in aqueous electrolyte systems),
SYS: @@ as well as some data for various solid phases (solution
SYS: @@ or stoichiometric) and a gaseous mixture phase.
SYS:
SYS: @@ For more Pourbaix diagram exercises, see TCEX40 and the
SYS: @@ extended examples TCEX40A to TCEX40E.
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: @@ Retrieve data from the PAQ2 database:
SYS: go data
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: rej sys
   ... the command in full is REJECT
 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
 REINITIATING GES .....
TDB_TCFE10: @@ Switch to the PAQ2 database
TDB_TCFE10: sw PAQ2
   ... the command in full is SWITCH_DATABASE
 Current database: Public Aqueous Soln (SIT) TDB v2.4

 H                       O                       ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                DIAMOND_A4              FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                CUB_A13                 CHI_A12
 FE4N                    FECN_CHI  REJECTED
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 PI  REJECTED
 FE3C                    NI3C                    CR3C2
 CR7C3                   CR23C6  REJECTED
 COCO3                   FECO3                   NAHCO3
 NA2CO3                  NA2CO3_S2               NICO3
 CRC6O6  REJECTED
 CO3N                    CRN                     CR2N
 FE2N                    NI3N  REJECTED
```

```
 NANO2                    NANO2_S2                 NANO3
   REJECTED
 COCL2                    CRCL2                    CRCL3
 FECL2                    FECL3                    NICL2
   REJECTED
 FECLO                    NACLO4                   NACLO4_S2
   REJECTED
TDB_PAQ2: data
   ... the command in full is DATABASE_INFORMATION
 Current database: Public Aqueous Soln (SIT) TDB v2.4

                                    PAQ2
             Thermo-Calc PUBLIC AQUEOUS DATABASE FOR POURBAIX MODULE
        (based on and replacing AQ in TCC/TCW & PAQ in TCC-Demo/TCW-Demo)
       ******************************************************************
                         (Version 2.4, Feb. 2008)
             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
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                    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
16:21:58,513 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 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-
16:21:58,925 WARN  The handling of the excess model command is not yet supported in GES6.
16:21:58,926 WARN  The handling of the add contribution command is not yet supported in GES6.
16:21:58,929 WARN  The handling of the fraction limits command is not yet supported in GES6.
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: @@ Define the system-components and the reference states:
TDB_PAQ2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: d-com H2O H+1 ZE Na Cl
   ... the command in full is DEFINE_COMPONENTS
POLY: s-r-s H2O AQUEOUS * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY: s-r-s ZE  REF_ELE * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY: 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:

POLY: @@ Define the equilibrium conditions
POLY: @@ ---------------------------------------------------------
POLY: @@ Define P-T and bulk composition in the interaction system
POLY: @@ for the calculations of initial equilibria:
POLY:
POLY: s-c P=1e5 T=298.15 b(H2O)=1000
   ... the command in full is SET_CONDITION
POLY: s-in-am b(Na1Cl1)=5
   ... the command in full is SET_INPUT_AMOUNTS
POLY: s-c n(H+1)=0 n(ZE)=0
   ... the command in full is SET_CONDITION
 Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
 Convergence in the equilibrium calculation can be hard to reach with zero amount conditions; It is recommended to suspend a component instead
POLY: 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:
POLY: @@ Calculate an equilibrium with only AQUEOUS:
POLY: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
```

```
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 AQUEOUS                  ENTERED      0.000000E+00    1.785600E+03
 SUSPENDED PHASES:
 REF_ELECTRODE NAOH_S2 NAOH NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O HCP_A3
 HALITE FCC_A1 BCC_A2 GAS
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated          1212 grid points in             0 s
Found the set of lowest grid points in              0 s
 Creating a new composition set AQUEOUS#2
 Calculated POLY solution       1 s, total time     1  s
POLY: 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#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00  Mole fractions:
 H2O  9.96927E-01  NA   1.53654E-03  H+1 -1.74641E-09
 CL   1.53654E-03  ZE   1.54532E-09
 Constitution:            SiteFraction    Molality      Activity    log10Act
 H2O                       9.96927E-01   5.55084E+01   9.96605E-01    -0.0015
 CL-1                      1.53654E-03   8.55538E-02   6.73425E-02    -1.1717
 NA+1                      1.53654E-03   8.55538E-02   6.73424E-02    -1.1717
 H+1                       2.37132E-09   1.32034E-07   1.04050E-07    -6.9828
 OH-1                      2.19965E-09   1.22476E-07   9.63757E-08    -7.0160
 O2                        4.70270E-10   2.61844E-08   2.61828E-08    -7.5820
 O3                        1.00000E-12   0.00000E+00   2.70935E-38   -37.5671
 HCLO                      1.00000E-12   0.00000E+00   3.25360E-20   -19.4876
 H2O2                      1.00000E-12   0.00000E+00   3.68420E-21   -20.4337
 HCLO2                     1.00000E-12   0.00000E+00   1.28717E-37   -36.8904
 H2                        1.00000E-12   0.00000E+00   5.39110E-43   -42.2683
 HO2-1                     1.00000E-12   0.00000E+00   7.49315E-26   -25.1253
 CLO4-1                    1.00000E-12   0.00000E+00   8.09139E-33   -32.0920
 CLO3-1                    1.00000E-12   0.00000E+00   1.41605E-30   -29.8489
 CLO2-1                    1.00000E-12   0.00000E+00   1.29472E-32   -31.8878
 CLO2                      1.00000E-12   0.00000E+00   4.84011E-38   -37.3151
 CLO-1                     1.00000E-12   0.00000E+00   6.77886E-21   -20.1688
 CL2                       1.00000E-12   0.00000E+00   4.80004E-25   -24.3188
 Solution Properties:   pH =   6.9828    Eh =    0.7417 V     I =   0.0856
                        pe =  12.5375    Ah =   71.5647 kJ   m* =   0.1711
                        Aw =   0.9966    Os =    1.1033     pKw =  13.9973
                        At1= 1.0000E-12  At2= 1.2248E-07 (equiv_mol/kg_H2O)
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 AQUEOUS#2                ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS#1                ENTERED      0.000000E+00    5.567954E+01
 SUSPENDED PHASES:
 REF_ELECTRODE NAOH_S2 NAOH NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O HCP_A3
 HALITE FCC_A1 BCC_A2 GAS
POLY: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.
 N=55.679543
 N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042549E-8,
    N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY:Hit RETURN to continue
POLY:
POLY: @@ Calculate an equilibrium with all phases (except for REF_ELE)
POLY:
POLY: c-st p *=ent 0
   ... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY:
POLY: @@ Always set the REF_ELECTRODE phase as SUSPENDED:
POLY:
POLY: c-st p REF_ELE=sus
   ... the command in full is CHANGE_STATUS
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 NAOH_S2                  ENTERED      0.000000E+00    0.000000E+00
 NAOH                     ENTERED      0.000000E+00    0.000000E+00
 NAO2                     ENTERED      0.000000E+00    0.000000E+00
 NA2O_S3                  ENTERED      0.000000E+00    0.000000E+00
 NA2O_S2                  ENTERED      0.000000E+00    0.000000E+00
 NA2O2_S2                 ENTERED      0.000000E+00    0.000000E+00
 NA2O2                    ENTERED      0.000000E+00    0.000000E+00
 NA2O                     ENTERED      0.000000E+00    0.000000E+00
 HCP_A3                   ENTERED      0.000000E+00    0.000000E+00
 HALITE                   ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                   ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                   ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS#2                ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS#1                ENTERED      0.000000E+00    5.580000E+01
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated           806 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: 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#1                   Status ENTERED     Driving force  0.0000E+00
 Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00  Mole fractions:
 H2O  9.96927E-01  NA   1.53654E-03  H+1 -1.74641E-09
 CL   1.53654E-03  ZE   1.54532E-09
 Constitution:           SiteFraction    Molality      Activity    log10Act
 H2O                      9.96927E-01   5.55084E+01   9.96605E-01    -0.0015
 CL-1                     1.53654E-03   8.55538E-02   6.73425E-02    -1.1717
 NA+1                     1.53654E-03   8.55538E-02   6.73424E-02    -1.1717
 H+1                      2.37132E-09   1.32034E-07   1.04050E-07    -6.9828
 OH-1                     2.19965E-09   1.22476E-07   9.63757E-08    -7.0160
 O2                       4.70270E-10   2.61844E-08   2.61828E-08    -7.5820
 O3                       1.00000E-12   0.00000E+00   2.70935E-38   -37.5671
 HCLO                     1.00000E-12   0.00000E+00   3.25360E-20   -19.4876
 H2O2                     1.00000E-12   0.00000E+00   3.68420E-21   -20.4337
 HCLO2                    1.00000E-12   0.00000E+00   1.28717E-37   -36.8904
 H2                       1.00000E-12   0.00000E+00   5.39110E-43   -42.2683
 HO2-1                    1.00000E-12   0.00000E+00   7.49315E-26   -25.1253
 CLO4-1                   1.00000E-12   0.00000E+00   8.09139E-33   -32.0920
 CLO3-1                   1.00000E-12   0.00000E+00   1.41605E-30   -29.8489
 CLO2-1                   1.00000E-12   0.00000E+00   1.29472E-32   -31.8878
 CLO2                     1.00000E-12   0.00000E+00   4.84011E-38   -37.3151
 CLO-1                    1.00000E-12   0.00000E+00   6.77886E-21   -20.1688
 CL2                      1.00000E-12   0.00000E+00   4.80004E-25   -24.3188
 Solution Properties:   pH =   6.9828    Eh =    0.7417 V     I =   0.0856
                        pe =  12.5375    Ah =   71.5647 kJ   m* =   0.1711
                        Aw =   0.9966    Os =    1.1033     pKw =  13.9973
                        At1= 1.0000E-12  At2= 1.2248E-07 (equiv_mol/kg_H2O)
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 AQUEOUS#2               ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS#1               ENTERED      0.000000E+00    5.567954E+01
 GAS                     ENTERED     -3.453482E+00    0.000000E+00
 HALITE                  ENTERED     -4.519288E+00    0.000000E+00
 NAOH                    ENTERED     -1.737487E+01    0.000000E+00
 BCC_A2                  ENTERED     -1.752962E+01    0.000000E+00
 FCC_A1                  ENTERED     -1.752962E+01    0.000000E+00
 NAOH_S2                 ENTERED     -1.793977E+01    0.000000E+00
 NAO2                    ENTERED     -1.999496E+01    0.000000E+00
 NA2O2                   ENTERED     -2.605088E+01    0.000000E+00
 NA2O2_S2                ENTERED     -2.640940E+01    0.000000E+00
 NA2O                    ENTERED     -4.241247E+01    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -4.257992E+01
 NA2O_S2 NA2O_S3 HCP_A3
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY: 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)=8.604255E-8,
    N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY:
POLY: @@ As shown here, 0.5wt% of NaCl (in 1 kg of H2O) is
POLY: @@ equivalent to 0.085554 molality of NaCl.
POLY:
POLY: @@ Save the workspace for the H2O-NaCl system:
POLY: save TCEX53_a.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continue
POLY:
POLY: @@ ==========================================================
POLY: @@ Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co)
POLY: @@ ==========================================================
POLY: @@ To demonstrate how to define the initial amount of alloy
POLY: @@ in an aqueous-bearing heterogeneous interaction system:
POLY: @@ ----------------------------------------------------------
POLY: @@  Note: We are only interested in the BCC_A2 and FCC_A1
POLY: @@   phases in the Fe-based alloy, in the current testing
POLY: @@   calculation. If necessary, you can consider other
POLY: @@   phases (which exist in the applied steel material).
POLY:
POLY: go data
   ... the command in full is GOTO_MODULE
TDB_PAQ2: rej sys
   ... the command in full is REJECT
 H                       O                       ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                DIAMOND_A4              FC_ORTHORHOMBIC
 MONOCLINIC  REJECTED
 CBCC_A12                CUB_A13                 CHI_A12
 FE4N                    FECN_CHI  REJECTED
 CEMENTITE               M23C6                   M7C3
 M5C2                    M3C2                    KSI_CARBIDE
 PI  REJECTED
 FE3C                    NI3C                    CR3C2
 CR7C3                   CR23C6  REJECTED
 COCO3                   FECO3                   NAHCO3
 NA2CO3                  NA2CO3_S2               NICO3
 CRC6O6  REJECTED
 CO3N                    CRN                     CR2N
```

```
 FE2N                    NI3N  REJECTED
 NANO2                   NANO2_S2                NANO3
   REJECTED
 COCL2                   CRCL2                   CRCL3
 FECL2                   FECL3                   NICL2
   REJECTED
 FECLO                   NACLO4                  NACLO4_S2
   REJECTED
 REINITIATING GES .....
TDB_PAQ2: sw PAQ2
   ... the command in full is SWITCH_DATABASE
TDB_PAQ2: rej ele H O ZE
   ... the command in full is REJECT
 H                       O                       ZE
   REJECTED
TDB_PAQ2: d-sys Fe Cr Ni Co
   ... the command in full is DEFINE_SYSTEM
 FE                      CR                      NI
 CO  DEFINED
TDB_PAQ2: l-sys const
   ... the command in full is LIST_SYSTEM
 GAS:G       :CO CR CR2 FE NI:
  > Gaseous Mixture, using the ideal gas model
 FCC_A1      :CO CR FE NI:VA:
  > This is also the MX (X=C,N) solution phase.
 BCC_A2      :CO CR FE NI:VA:
  > This is also the MX3 (X=C,N) solution phase.
 HCP_A3      :CO CR FE NI:VA:
  > This is also the M2X (X=C,N) solution phase.
 SIGMA       :CO FE NI:CR:CO CR FE NI:
TDB_PAQ2: rej-ph *
   ... the command in full is REJECT
 GAS:G                   FCC_A1                  BCC_A2
 HCP_A3                  SIGMA  REJECTED
TDB_PAQ2: rest-ph FCC_A1 BCC_A2
   ... the command in full is RESTORE
 FCC_A1                  BCC_A2  RESTORED
TDB_PAQ2: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
   ... the command in full is AMEND_PHASE_DESCRIPTION
   ... the command in full is AMEND_PHASE_DESCRIPTION
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
      -Cr-Na-Ni-C-H-O-N-S-Cl system.'
 -OK-
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY:
POLY: @@ You can turn on the Global Minimization:
POLY: Adv-Opt EQ_CALC Y Y !
   ... the command in full is ADVANCED_OPTIONS
 Settings for the minimization of an equilibra:
POLY: Adv-Opt GLOBAL  Y 20000 !
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY:
POLY: s-c P=1e5 T=298.15
   ... the command in full is SET_CONDITION
POLY:
POLY: @@ The following conditions [system-size B and initial bulk
POLY: @@ composition w(i) of Fe-alloy] corresponds to the total
POLY: @@ initial amount of Fe-based alloy in the interaction,
POLY: @@ i.e., 1 gram of steel (Fe-10Cr-5Ni-1Co wt%).
POLY:
POLY: s-c B=1  w(Cr)=.10 w(Ni)=.05 w(Co)=.01
   ... the command in full is SET_CONDITION
POLY:
POLY: 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: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         39232 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
 Creating a new composition set BCC_A2#3
POLY: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.79859E-02,  Mass in grams  1.00000E+00
 Total Gibbs energy -1.58616E+02,  Enthalpy -1.09888E+01,  Volume  0.00000E+00

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 CO                      1.6968E-04  9.4342E-03 4.4157E-08 -4.1983E+04 SER
 CR                      1.9232E-03  1.0693E-01 5.8926E-02 -7.0192E+03 SER
 FE                      1.5041E-02  8.3627E-01 3.7073E-02 -8.1679E+03 SER
 NI                      8.5193E-04  4.7367E-02 7.7089E-04 -1.7769E+04 SER

 BCC_A2#3                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.4641E-02, Mass 8.1821E-01, Volume fraction 0.0000E+00  Mole fractions:
 FE  9.87131E-01  CO  1.15888E-02  NI  8.17873E-04  CR  4.61992E-04

 BCC_A2#1                    Status ENTERED     Driving force  0.0000E+00
```

```
 Moles 1.9166E-03, Mass 9.9654E-02, Volume fraction 0.0000E+00  Mole fractions:
 CR  9.99946E-01  FE  5.39522E-05  CO  9.25541E-12  NI  8.81026E-12

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.4280E-03, Mass 8.2138E-02, Volume fraction 0.0000E+00  Mole fractions:
 NI  5.88202E-01  FE  4.11792E-01  CO  5.30943E-06  CR  6.98908E-09
POLY: l-st cp
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 CO                       ENTERED   SER
 CR                       ENTERED   SER
 FE                       ENTERED   SER
 NI                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    1.428010E-03
 BCC_A2#3                 ENTERED      0.000000E+00    1.464136E-02
 BCC_A2#2                 ENTERED      0.000000E+00    0.000000E+00
 BCC_A2#1                 ENTERED      0.000000E+00    1.916564E-03
POLY: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1.
 N=1.7985937E-2
 N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY:Hit RETURN to continue
POLY:
POLY: s-c T=1073.15
   ... the command in full is SET_CONDITION
POLY: l-c
   ... the command in full is LIST_CONDITIONS
 P=1E5, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Using global minimization procedure
Calculated         39232 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: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
 DEGREES OF FREEDOM 0

 Temperature   1073.15 K (   800.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.79859E-02,  Mass in grams  1.00000E+00
 Total Gibbs energy -9.18150E+02,  Enthalpy  5.59650E+02,  Volume  0.00000E+00

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 CO                       1.6968E-04  9.4342E-03 1.8364E-05 -9.7303E+04 SER
 CR                       1.9232E-03  1.0693E-01 3.0133E-03 -5.1794E+04 SER
 FE                       1.5041E-02  8.3627E-01 4.2352E-03 -4.8757E+04 SER
 NI                       8.5193E-04  4.7367E-02 1.1925E-04 -8.0610E+04 SER

 FCC_A1                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.7986E-02, Mass 1.0000E+00, Volume fraction 0.0000E+00  Mole fractions:
 FE  8.36270E-01  CR  1.06929E-01  NI  4.73667E-02  CO  9.43424E-03
POLY: l-st cp
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL COMPONENTS
 COMPONENT                STATUS    REF. STATE     T(K)           P(Pa)
 VA                       ENTERED   SER
 CO                       ENTERED   SER
 CR                       ENTERED   SER
 FE                       ENTERED   SER
 NI                       ENTERED   SER
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 FCC_A1                   ENTERED      0.000000E+00    1.798594E-02
 BCC_A2#3                 ENTERED     -1.564120E-02    0.000000E+00
 BCC_A2#2                 ENTERED     -1.564120E-02    0.000000E+00
 BCC_A2#1                 ENTERED     -1.564120E-02    0.000000E+00
POLY: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1.
 N=1.7985937E-2
 N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY: @@
POLY: @@ As shown here, 1 gram of steel (Fe-10Cr-5Ni-1Co wt%)
POLY: @@ is equivalent to:
POLY: @@       n(Fe) = 1.5041094E-2
POLY: @@       n(Cr) = 1.9232249E-3
POLY: @@       n(Ni) = 8.5193389E-4
POLY: @@       n(Co) = 1.6968422E-4
POLY:
POLY: @@ Save the workspace for the Fe-Cr-Ni-Co system:
POLY: save TCEX53_b.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continue
POLY:
POLY: @@ ==========================================================
POLY: @@ Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl
POLY: @@ ==========================================================
POLY: @@ Bulk composition in the heterogeneous interaction system:
POLY: @@          b(H2O)  = 1000
POLY: @@          n(NaCl) = 0.085554
POLY: @@          n(Fe) = 1.5041094E-2
POLY: @@          n(Cr) = 1.9232249E-3
POLY: @@          n(Ni) = 8.5193389E-4
POLY: @@          n(Co) = 1.6968422E-4
POLY:
POLY: @@ Retrieve data from the PAQ2 database:
POLY: go data
   ... the command in full is GOTO_MODULE
TDB_PAQ2: rej sys
   ... the command in full is REJECT
 H                        O                       ZE
 VA  DEFINED
 LIQUID:L  REJECTED
 GRAPHITE                 DIAMOND_A4              FC_ORTHORHOMBIC
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```
 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 GES .....
TDB_PAQ2: @@ Switch to the PAQ2 database
TDB_PAQ2: sw PAQ2
   ... the command in full is SWITCH_DATABASE
TDB_PAQ2: d-sys H O Na Cl Fe Cr Ni Co
   ... the command in full is DEFINE_SYSTEM
 NA                      CL                      FE
 CR                      NI                      CO
   DEFINED
TDB_PAQ2: l-sys const
   ... the command in full is LIST_SYSTEM
 AQUEOUS:A   :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CO1H2O2 CL2 CL-1 CLO2 CLO-1
  CLO2-1 CLO3-1 CLO4-1 HCLO HCLO2 CO+2 CO+3 CR+2 CR+3 CROH+2 CRO+1 CRO2-1
  HCRO2 HCRO4-1 CRO4-2 CR2O7-2 FE+2 FE+3 FEOH+1 FEOH+2 FEO3H3-1 FE2O2H2+4
  FECL+2 NA+1 NI+2 NIOH+1:
  > Aqueous Solution: using the SIT Model (from TCAQ2 database)
 REF_ELECTRODE :ZE:
  > Reference Electrode for ZE potentail; always SUSPENDED in POLY.
 GAS:G       :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1CO1 CL1CR1 CL1CR1O1
  CL1CR1O2 CL1FE1 CL1NA1 CL1NI1 CL2CO1 CL2CR1 CL2CR1O1 CL2CR1O2 CL2FE1
  CL2NA2 CL2NI1 CL3CO1 CL3CR1 CL3CR1O1 CL3FE1 CL3NA3 CL4CO2 CL4CR1 CL4CR1O1
  CL4FE2 CL5CR1 CL6CR1 CL6FE2 CO CO1H1 CO1H2O2 CO1O1 CR CR1H1 CR1H1O1
  CR1H1O2 CR1H1O3 CR1H2O2 CR1H2O3 CR1H2O4 CR1H3O3 CR1H3O4 CR1H4O4 CR1H4O5
  CR1O1 CR1O2 CR1O3 CR2 CR2O1 CR2O2 CR2O3 FE FE1H1O1 FE1H1O2 FE1H2O2 FE1O1
  FE1O2 H H1NA1 H1NA1O1 H1NI1 H1NI1O1 H1O1 H1O2 H2 H2NA2O2 H2NI1O2 H2O1 H2O2
  NA NA1O1 NA2 NA2O1 NA2O2 NI NI1O1 O O2 O3:
  > Gaseous Mixture, using the ideal gas model
 FCC_A1      :CO CR FE NA NI O:VA:
  > This is also the MX (X=C,N) solution phase.
 BCC_A2      :CO CR FE NA NI O:VA:
  > This is also the MX3 (X=C,N) solution phase.
 HCP_A3      :CO CR FE NA NI:VA:
  > This is also the M2X (X=C,N) solution phase.
 SIGMA       :CO FE NI:CR:CO CR FE NI:
 HALITE      :NA1CL1:
 WUSTITE     :FE0.947O1:
 MAGNETITE   :FE3O4:
 HEMATITE    :FE2O3:
 FE2O3_GAMMA :FE2O3:
 FEO2H2      :FE1H2O2:
 FEO3H3      :FE1H3O3:
 FEOOH       :FE1H1O2:
 FE2O2O2H2   :FE2H2O4:
 COO         :CO1O1:
 CO3O4       :CO3O4:
 COO2H2      :CO1H2O2:
 CRO2        :CR1O2:
 CRO3        :CR1O3:
 CR2O3       :CR2O3:
 CR5O12      :CR5O12:
 CR8O21      :CR8O21:
 NAO2        :NA1O2:
 NA2O        :NA2O1:
 NA2O_S2     :NA2O1:
 NA2O_S3     :NA2O1:
 NA2O2       :NA2O2:
 NA2O2_S2    :NA2O2:
 NAOH        :H1NA1O1:
 NAOH_S2     :H1NA1O1:
 NIO         :NI1O1:
 NIO_S2      :NI1O1:
 NIO2H2      :H2NI1O2:
 NIOOH       :H1NI1O2:
 FECR2O4     :CR2FE1O4:
 COCR2O4     :CO1CR2O4:
 NICR2O4     :CR2NI1O4:
 NA2CR2O4    :CR2NA2O4:
 COFE2O4     :CO1FE2O4:
 NIFE2O4     :FE2NI1O4:
 NA2CRO4     :CR1NA2O4:
 NA2CRO4_S2  :CR1NA2O4:
 NA2FEO2     :FE1NA1O2:
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: rej ph  HCP_A3 CBCC_A12 CUB_A13 CHI_A12 Fe4N
   ... the command in full is REJECT
 HCP_A3  REJECTED
TDB_PAQ2: rej ph  SIGMA
   ... the command in full is REJECT
 SIGMA  REJECTED
TDB_PAQ2: rej ph  NaH
   ... the command in full is REJECT
TDB_PAQ2: get
   ... the command in full is GET_DATA
 REINITIATING GES .....
 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 ...
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 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-
16:22:02,799 WARN  The handling of the excess model command is not yet supported in GES6.
16:22:02,801 WARN  The handling of the add contribution command is not yet supported in GES6.
16:22:02,804 WARN  The handling of the fraction limits command is not yet supported in GES6.
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: @@ Define system-components and the reference states:
TDB_PAQ2: go p-3
   ... the command in full is GOTO_MODULE

 POLY version  3.32
POLY: d-com H2O H+1 ZE Na Cl Fe Cr Ni Co
   ... the command in full is DEFINE_COMPONENTS
POLY: s-r-s H2O AQUEOUS * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY: s-r-s ZE  REF_ELE * 1e5
   ... the command in full is SET_REFERENCE_STATE
POLY: 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:
POLY: @@ Define some symbols (constants/variables/functions/tables):
POLY: @@ You can define some important ones e.g., RNF; pH, Eh
POLY: @@ ==========================================================
POLY: @@ Important: With the default reference state (SER) used for
POLY: @@ system-component H+1, the pH condition in aqueous solution
POLY: @@ should be defined as:
POLY: @@     pH = -log10[act(H+1,aqs)] (traditional)
POLY: @@        = -log10[acr(H+1,AQUEOUS)*55.508435] (Thermo-Calc)
POLY: @@        = -ln[acr(H+1,AQUEOUS)*55.508435]*2.302585093
POLY: @@  where
POLY: @@    act(H+1,aqs) is molality_based activity of
POLY: @@        H+1 species (as of the traditional concept);
POLY: @@    acr(H+1,AQ)*AH2O is site-fraction_based activity of
POLY: @@        H+1 species (calculated in Thermo-Calc).
POLY: @@
POLY: @@  Such a definition not only gives correct pH values for all
POLY: @@  thermodynamic models (SIT and HKF) but also does not affect
POLY: @@  the calculation of ACR(H+1) [LNACR(H+1)] quantity that is
POLY: @@  normally used as MAPPING/STEPPING variables in all modules
POLY: @@  (POURBAIX & TDB/GES5/POLY3/POST).
POLY: @@ ==========================================================
POLY:
POLY: @@ You can also choose to define many other symbols (for
POLY: @@ plotting) on the same scope of the POURBAIX module.
POLY:
POLY: @@ A list of valid symbols for the Fe-Cr-Ni-Co-H2O-NaCl
POLY: @@ heterogeneous interaction system on the scope same as the
POLY: @@ automatically defined symbols in the POURBAIX module can be
POLY: @@ found at the end of this MACRO file (but only as a reference).
POLY: @@ ----------------------------------------------------------
POLY: @@ It is important to note that:
POLY: @@ * AH2O is always a constant, and YH2O is the site fraction
POLY: @@   of the solvent H2O, i.e.,
POLY: @@      AH2O = 55.508435
POLY: @@      YH2O = Y(AQ,H2O)
POLY:
POLY: @@ * The AYT and ART quantities are on the Site-Fraction basis:
POLY: @@      AYT for AC(i,AQ)
POLY: @@      ART for ACR(i,AQ)
POLY:
POLY: @@ * The AIT (AIi), RCT (RCi) and MLT (MLi) quantities are
POLY: @@   on the Molality basis:
POLY: @@      AIT for ACR(i,AQ)*AH2O
POLY: @@          as activity based on molality
POLY: @@      RCT for ACR(i,AQ)*YH2O/Y(AQ,i)
POLY: @@          as activity coefficient based on molality
POLY: @@      MLT for Y(AQ,i)*AH2O/YH2O
POLY: @@          as molality
POLY: @@ ----------------------------------------------------------
POLY: @@      AIi = RCi * MLi
POLY: @@          = ACR(i,AQ)*YH2O/Y(AQ,i) * Y(AQ,i)*AH2O/YH2O
POLY: @@          = ACR(i,AQ)*AH2O
POLY:
POLY: @@ * It is always ACR(sp,AQ) = AC(sp,AQ)
POLY:
POLY: @@ * It is always the AIi=AIT(H+1) [=ACR(H+1,AQ)*AH2O]
POLY: @@   quantity, rather than ART(H+1) [=ACR(H+1,AQ)] quantity,
POLY: @@   that is the equivalent property for the acidity
POLY: @@   condition pH.
POLY: @@ ----------------------------------------------------------
POLY:
POLY: ent-sym const AH2O=55.508435
   ... the command in full is ENTER_SYMBOL
POLY: ent-sym const RNF =96485.309
   ... the command in full is ENTER_SYMBOL
POLY: ent-sym funct Eh = mur(ZE)/RNF;
```

```
   ... the command in full is ENTER_SYMBOL
POLY: ent-sym funct pH = -log10(acr(H+1,AQUEOUS)*AH2O);
   ... the command in full is ENTER_SYMBOL
POLY: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED CONSTANTS
    AH2O=55.508435, RNF=96485.309
 DEFINED FUNCTIONS AND VARIABLES%
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
POLY:
POLY: @@ Define the equilibrium conditions:
POLY: @@ ----------------------------------------------------------
POLY: @@ Define P-T and bulk composition in the interaction system
POLY: @@ for calculating starting point [at e.g pH=7 & Eh=0 (V)]:
POLY:
POLY: @@ P-T conditions:
POLY: s-c P=1e5 T=298.15
   ... the command in full is SET_CONDITION
POLY: @@
POLY: @@ Alternatively, it can be manually input as below:
POLY: @@   s-c P=
POLY: @@ @?Pressure_in_Pascal:
POLY: @@   s-c T=
POLY: @@ @?Temperature_In_Kelvin:
POLY:
POLY: @@ For Aqueous-involving interaction systems, it is always
POLY: @@ recommended to define 1 kg of H2O, so that it is
POLY: @@ convenient to consider molality quantities and other
POLY: @@ properties in aqueous solution.
POLY:
POLY: s-c b(H2O)=1000
   ... the command in full is SET_CONDITION
POLY:
POLY: @@ The following is equivalent to 0.085554 mole of NaCl
POLY: @@ in 1 kg of H2O:
POLY: s-c n(Na)=0.085554  n(Cl)=0.085554
   ... the command in full is SET_CONDITION
POLY:
POLY: @@ For calculating Pourbaix diagrams or other diagrams in
POLY: @@ aqueous-involving interaction system, it is important
POLY: @@ to consider the so-called "effective interaction rate".
POLY:
POLY: @@ The following is equivalent to 1 gram of specified
POLY: @@ steel (Fe-10Cr-5Ni-1Co wt%) in an effective interaction
POLY: @@ with 1 kg of H2O (dissolving 0.085554 mole of NaCl):
POLY:
POLY: s-c n(Fe)=1.5041094E-2  n(Cr)=1.9232249E-3
   ... the command in full is SET_CONDITION
POLY: s-c n(Ni)=8.5193389E-4  n(Co)=1.6968422E-4
   ... the command in full is SET_CONDITION
POLY:
POLY: @@ Let's calculate initial equilibrium at pH=7 & Eh=0 (V):
POLY: s-c lnacr(H+1)=-16.11809565  mur(ZE)=0
   ... the command in full is SET_CONDITION
POLY:
POLY: 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:
POLY: @@ ==========================================================
POLY: @@ Turn off GLOBAL completely for aqueous calculations
POLY: @@ ----------------------------------------------------------
POLY: @@   Adv-Opt GLOBAL
POLY: @@   Use global minimization as much as possible /N/: N
POLY: @@   Use global minimization for test only? /N/:      N
POLY: @@ -------------------------------------------------------
POLY: @@
POLY: Adv-Opt GLOBAL N N !
   ... the command in full is ADVANCED_OPTIONS
 Settings for global minimization:
POLY: @@
POLY: @@ ----------------------------------------------------------
POLY: @@  Adv-Opt EQ_CALC
POLY: @@   Force positive definite phase Hessian /Y/:      N
POLY: @@   Control stepsize during minimization /Y/:       Y
POLY: @@ ----------------------------------------------------------
POLY: Adv-Opt EQ_CALC N Y !
   ... the command in full is ADVANCED_OPTIONS
 Settings for the minimization of an equilibra:
POLY:
POLY: @@ ==========================================================
POLY: @@ Set numerical limits:
POLY: @@ ----------------------------------------------------------
POLY: @@  Notes:
POLY: @@  For equilibrium calculations (single-point, stepping or
POLY: @@  mapping) of complex aqueous-bearing heterogeneous
POLY: @@  interaction systems, it is recommended to modify the
POLY: @@  numerical limits.
POLY:
POLY: @@  The next command (changing the numerical limits from the
POLY: @@  default values "500 1E-6 1E-12 N" to "20000 1E-6 1E-20 Y")
POLY: @@  makes the following changes:


POLY: @@  1) Changes "Maximum number of iterations" from the
POLY: @@     default 500 to 20000, which enforces 40 times more
POLY: @@     iterations for each of the calculations in order
POLY: @@     to obtain stable equilibria;
POLY: @@  2) The "Required accuracy" remains the default value 1E-6.
POLY: @@     It can be changed to 1E-4, that allows less accurate
POLY: @@     calculations but makes it easier/faster to converge;
POLY: @@  3) Changes "Smallest fraction" from the default site
POLY: @@     fraction of 1E-12 to 1E-20, which is more suitable
POLY: @@     for aqueous solution phases; and
POLY: @@  4) The "Approximate driving force for metastable phases"
POLY: @@     is changed from the default of "N" to "Y" (meaning
POLY: @@     it should always approximately calculate driving
```

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POLY: @@     forces for metastable phases).
POLY:
POLY: @@ These changes in the numerical limits are essential and
POLY: @@ useful for making sure of finding a converged solution of
POLY: @@ stable equilbria, especially when the heterogeneous
POLY: @@ interaction system becomes more complicated.
POLY: @@ ---------------------------------------------------------
POLY:
POLY: s-n-l 20000 1e-6 1e-20 Y
   ... the command in full is SET_NUMERICAL_LIMITS
 LIMITATIONS of the present version of Thermo-Calc
 Max number of elements                      :  80
 Max number of species                       :5000
 Max number of sublattices in a phase        :  10
 Max number of constituents in a phase:      : 200
 Max number of constituents in an ideal phase :5000
POLY:
POLY:
POLY: @@ Calculate an equilibrium with only AQUEOUS:
POLY: c-st p *=sus
   ... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 AQUEOUS                  ENTERED      0.000000E+00    6.138000E+03
 SUSPENDED PHASES:
 WUSTITE REF_ELECTRODE NIO_S2 NIOOH NIO2H2 NIO NIFE2O4 NICR2O4 NAOH_S2 NAOH
 NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O NA2FEO2 NA2CRO4_S2 NA2CRO4 NA2CR2O4
 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4 FE2O3_GAMMA FE2O2O2H2
 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO2H2 COO COFE2O4 COCR2O4 CO3O4 BCC_A2
 GAS
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM
 Global equilibrium calculation turned off, you can turn it on with
 ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,
   109 ITS,  CPU TIME USED   0 SECONDS
POLY: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
    LNACR(H+1)=-16.1181, MUR(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.57254E+01,  Mass in grams  1.00599E+03
 Total Gibbs energy -1.70641E+07,  Enthalpy -1.59024E+07,  Volume -4.21624E-08

 Component               Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                     5.5508E+01  9.9611E-01 9.9606E-01 -9.7846E+00 AQUEOUS
 H+1                    -1.0027E-02 -1.7993E-04 1.0000E-07 -3.9956E+04 SER
 ZE                      3.7895E-02  6.8003E-04 1.0000E+00  0.0000E+00 REF_ELEC
 NA                      8.5554E-02  1.5353E-03 1.5211E-50 -2.8436E+05 SER
 CL                      8.5554E-02  1.5353E-03 1.1822E-30 -1.7083E+05 SER
 FE                      1.5041E-02  2.6991E-04 1.2285E-18 -1.0223E+05 SER
 CR                      1.9232E-03  3.4513E-05 1.6596E-45 -2.5561E+05 SER
 NI                      8.5193E-04  1.5288E-05 6.0058E-14 -7.5468E+04 SER
 CO                      1.6968E-04  3.0450E-06 3.2708E-16 -8.8391E+04 SER

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5725E+01, Mass 1.0060E+03, Volume fraction 1.0000E+00  Mole fractions:
 H2O  9.96107E-01  ZE   6.80033E-04  NI   1.52881E-05
 CL   1.53528E-03  FE   2.69915E-04  CO   3.04501E-06
 NA   1.53528E-03  CR   3.45125E-05  H+1 -1.79930E-04
 Constitution:           SiteFraction    Molality      Activity    log10Act
 H2O                      9.96604E-01   5.55084E+01   9.96157E-01    -0.0017
 NA+1                     1.53628E-03   8.55668E-02   6.59591E-02    -1.1807
 CL-1                     1.53628E-03   8.55668E-02   6.59412E-02    -1.1808
 FE+2                     1.56791E-04   8.73285E-03   3.08751E-03    -2.5104
 FEOH+1                   1.13299E-04   6.31049E-03   4.86919E-03    -2.3125
 CRO+1                    3.00740E-05   1.67505E-03   1.29247E-03    -2.8886
 NI+2                     1.52852E-05   8.51348E-04   3.02381E-04    -3.5194
 CROH+2                   3.38456E-06   1.88512E-04   6.68399E-05    -4.1750
 CO+2                     3.04698E-06   1.69710E-04   6.02711E-05    -4.2199
 HCRO2                    1.05903E-06   5.89856E-05   5.89799E-05    -4.2293
 NIOH+1                   1.28111E-08   7.13548E-07   5.50574E-07    -6.2592
 CR+3                     1.12056E-08   6.24122E-07   6.07385E-08    -7.2165
 CRO2-1                   6.16631E-09   3.43448E-07   2.65005E-07    -6.5767
 OH-1                     2.33522E-09   1.30066E-07   1.00231E-07    -6.9990
 H+1                      2.32641E-09   1.29576E-07   1.00000E-07    -7.0000
 FEOH+2                   1.10316E-12   6.14435E-11   2.17858E-11   -10.6618
 CR+2                     1.47493E-16   8.21498E-15   2.91275E-15   -14.5357
 FE+3                     6.69156E-17   3.72704E-15   3.61605E-16   -15.4418
 FECL+2                   3.43228E-17   1.91170E-15   6.77823E-16   -15.1689
 H2                       1.06276E-19   5.91933E-18   5.91876E-18   -17.2278
 FE2O2H2+4                2.32944E-20   1.29744E-18   2.05117E-20   -19.6880
 O2                       1.00000E-20   5.56976E-19   2.17014E-58   -57.6635
 FEO3H3-1                 1.00000E-20   5.56976E-19   4.15261E-44   -43.3817
 H2O2                     1.00000E-20   5.56976E-19   3.35251E-46   -45.4746
 CRO4-2                   1.00000E-20   5.56976E-19   1.67197E-26   -25.7768
 HCLO                     1.00000E-20   5.56976E-19   2.78756E-45   -44.5548
 HCLO2                    1.00000E-20   5.56976E-19   1.00400E-87   -86.9983
 CR2O7-2                  1.00000E-20   5.56976E-19   9.28118E-52   -51.0324
 HCRO4-1                  1.00000E-20   5.56976E-19   5.05292E-27   -26.2965
 HO2-1                    1.00000E-20   5.56976E-19   7.09471E-51   -50.1491
 CO1H2O2                  1.00000E-20   5.56976E-19   5.9656E-101  -100.2243
 CO+3                     1.00000E-20   5.56976E-19   7.96270E-38   -37.0989
 O3                       1.00000E-20   5.56976E-19   2.0444E-113  -112.6894
 CLO4-1                   1.00000E-20   5.56976E-19   5.4430E-133  -132.2642
 CLO3-1                   1.00000E-20   5.56976E-19   1.0463E-105  -104.9803
 CLO2-1                   1.00000E-20   5.56976E-19   1.05079E-82   -81.9785
 CLO2                     1.00000E-20   5.56976E-19   1.1394E-100   -99.9433
 CLO-1                    1.00000E-20   5.56976E-19   6.04311E-46   -45.2187
 CL2                      1.00000E-20   5.56976E-19   3.87204E-50   -49.4121
 Solution Properties:   pH =   7.0000    Eh =    0.0000 V     I =   0.1094
                        pe =   0.0000    Ah =    0.0000 kJ   m* =   0.1891
                        Aw =   0.9962    Os =    1.1300     pKw =  13.9973
                        At1= 1.0000E-20  At2= 1.3007E-07 (equiv_mol/kg_H2O)
POLY: l-st p
   ... the command in full is LIST_STATUS
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 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 AQUEOUS                  ENTERED      0.000000E+00    5.572540E+01
 SUSPENDED PHASES:
 WUSTITE REF_ELECTRODE NIO_S2 NIOOH NIO2H2 NIO NIFE2O4 NICR2O4 NAOH_S2 NAOH
 NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O NA2FEO2 NA2CRO4_S2 NA2CRO4 NA2CR2O4
 MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4 FE2O3_GAMMA FE2O2O2H2
 FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO2H2 COO COFE2O4 COCR2O4 CO3O4 BCC_A2
 GAS
POLY: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.9899
 N=55.725397
 N(H2O)=55.508435, N(H+1)=-1.0026646E-2, N(ZE)=3.7895099E-2, N(NA)=8.5554E-2,
    N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
    N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY:Hit RETURN to continuePOLY:
POLY: @@ Calculate an equilibrium with all phases (except for REF_ELE):
POLY:
POLY: c-st p *=ent 0
   ... the command in full is CHANGE_STATUS
POLY: c-st p AQUEOUS=ent 55.8
   ... the command in full is CHANGE_STATUS
POLY: @@ Always set the REF_ELECTRODE phase as SUSPENDED:
POLY: c-st p REF_ELE=sus
   ... the command in full is CHANGE_STATUS
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 WUSTITE                  ENTERED      0.000000E+00    0.000000E+00
 NIO_S2                   ENTERED      0.000000E+00    0.000000E+00
 NIOOH                    ENTERED      0.000000E+00    0.000000E+00
 NIO2H2                   ENTERED      0.000000E+00    0.000000E+00
 NIO                      ENTERED      0.000000E+00    0.000000E+00
 NIFE2O4                  ENTERED      0.000000E+00    0.000000E+00
 NICR2O4                  ENTERED      0.000000E+00    0.000000E+00
 NAOH_S2                  ENTERED      0.000000E+00    0.000000E+00
 NAOH                     ENTERED      0.000000E+00    0.000000E+00
 NAO2                     ENTERED      0.000000E+00    0.000000E+00
 NA2O_S3                  ENTERED      0.000000E+00    0.000000E+00
 NA2O_S2                  ENTERED      0.000000E+00    0.000000E+00
 NA2O2_S2                 ENTERED      0.000000E+00    0.000000E+00
 NA2O2                    ENTERED      0.000000E+00    0.000000E+00
 NA2O                     ENTERED      0.000000E+00    0.000000E+00
 NA2FEO2                  ENTERED      0.000000E+00    0.000000E+00
 NA2CRO4_S2               ENTERED      0.000000E+00    0.000000E+00
 NA2CRO4                  ENTERED      0.000000E+00    0.000000E+00
 NA2CR2O4                 ENTERED      0.000000E+00    0.000000E+00
 MAGNETITE                ENTERED      0.000000E+00    0.000000E+00
 HEMATITE                 ENTERED      0.000000E+00    0.000000E+00
 HALITE                   ENTERED      0.000000E+00    0.000000E+00
 FEOOH                    ENTERED      0.000000E+00    0.000000E+00
 FEO3H3                   ENTERED      0.000000E+00    0.000000E+00
 FEO2H2                   ENTERED      0.000000E+00    0.000000E+00
 FECR2O4                  ENTERED      0.000000E+00    0.000000E+00
 FE2O3_GAMMA              ENTERED      0.000000E+00    0.000000E+00
 FE2O2O2H2                ENTERED      0.000000E+00    0.000000E+00
 FCC_A1                   ENTERED      0.000000E+00    0.000000E+00
 CRO3                     ENTERED      0.000000E+00    0.000000E+00
 CRO2                     ENTERED      0.000000E+00    0.000000E+00
 CR8O21                   ENTERED      0.000000E+00    0.000000E+00
 CR5O12                   ENTERED      0.000000E+00    0.000000E+00
 CR2O3                    ENTERED      0.000000E+00    0.000000E+00
 COO2H2                   ENTERED      0.000000E+00    0.000000E+00
 COO                      ENTERED      0.000000E+00    0.000000E+00
 COFE2O4                  ENTERED      0.000000E+00    0.000000E+00
 COCR2O4                  ENTERED      0.000000E+00    0.000000E+00
 CO3O4                    ENTERED      0.000000E+00    0.000000E+00
 BCC_A2                   ENTERED      0.000000E+00    0.000000E+00
 AQUEOUS                  ENTERED      0.000000E+00    5.583623E+01
 GAS                      ENTERED      0.000000E+00    0.000000E+00
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY: c-e
   ... the command in full is COMPUTE_EQUILIBRIUM

    78 ITS,  CPU TIME USED   1 SECONDS
POLY: l-e ,x
   ... the command in full is LIST_EQUILIBRIUM
 Output from POLY-3, equilibrium =     1, label A0  , database: PAQ2

 Conditions:
 P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
    LNACR(H+1)=-16.1181, MUR(ZE)=0
 DEGREES OF FREEDOM 0

 Temperature    298.15 K (    25.00 C),  Pressure  1.000000E+05
 Number of moles of components  5.56976E+01,  Mass in grams  1.00595E+03
 Total Gibbs energy -1.70627E+07,  Enthalpy -1.59010E+07,  Volume -3.10120E-16

 Component                Moles       M-Fraction  Activity   Potential  Ref.stat
 H2O                      5.5508E+01  9.9660E-01 9.9654E-01 -8.5924E+00 AQUEOUS
 H+1                     -5.2910E-02 -9.4995E-04 1.0000E-07 -3.9956E+04 SER
 ZE                       5.2936E-02  9.5042E-04 1.0000E+00 -4.4035E-12 REF_ELEC
 NA                       8.5554E-02  1.5360E-03 1.5537E-50 -2.8431E+05 SER
 CL                       8.5554E-02  1.5360E-03 1.2078E-30 -1.7077E+05 SER
 FE                       1.5041E-02  2.7005E-04 5.2232E-26 -1.4431E+05 SER
 CR                       1.9232E-03  3.4530E-05 1.2572E-53 -3.0196E+05 SER
 NI                       8.5193E-04  1.5296E-05 1.0073E-15 -8.5603E+04 SER
 CO                       1.6968E-04  3.0465E-06 1.5331E-20 -1.1310E+05 SER

 AQUEOUS                     Status ENTERED     Driving force  0.0000E+00
 Moles 5.5653E+01, Mass 1.0045E+03, Volume fraction 1.0000E+00  Mole fractions:
 H2O  9.96925E-01  ZE   4.72606E-07  FE   1.08577E-11
 CL   1.53727E-03  NI   2.36161E-07  CR   2.55062E-13
 NA   1.53727E-03  CO   1.31447E-10  H+1 -2.25543E-10
 Constitution:           SiteFraction    Molality      Activity    log10Act
 H2O                      9.96925E-01   5.55084E+01   9.96603E-01    -0.0015
 CL-1                     1.53727E-03   8.55948E-02   6.73703E-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
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 NIOH+1                    2.10599E-10   1.17261E-08   9.23842E-09    -8.0344
 CO+2                      1.31447E-10   7.31890E-09   2.82496E-09    -8.5490
 FE+2                      6.13590E-12   3.41645E-10   1.31278E-10    -9.8818
 FEOH+1                    4.72178E-12   2.62907E-10   2.07132E-10    -9.6838
 CRO+1                     2.23303E-13   1.24334E-11   9.79571E-12   -11.0090
 CROH+2                    2.36100E-14   1.31459E-12   5.06585E-13   -12.2953
 HCRO2                     8.03267E-15   4.47256E-13   4.47228E-13   -12.3495
 CR+3                      7.04094E-17   3.92037E-15   4.60120E-16   -15.3371
 CRO2-1                    4.58077E-17   2.55056E-15   2.00946E-15   -14.6969
 H2                        1.06307E-19   5.91913E-18   5.91876E-18   -17.2278
 FEOH+2                    4.31923E-20   2.40493E-18   9.26752E-19   -18.0330
 O3                        1.00000E-20   0.00000E+00   2.0474E-113  -112.6888
 FEO3H3-1                  1.00000E-20   0.00000E+00   1.76819E-51   -50.7525
 FECL+2                    1.00000E-20   0.00000E+00   2.94449E-23   -22.5310
 FE2O2H2+4                 1.00000E-20   0.00000E+00   3.71178E-35   -34.4304
 FE+3                      1.00000E-20   0.00000E+00   1.53750E-23   -22.8132
 H2O2                      1.00000E-20   0.00000E+00   3.35574E-46   -45.4742
 HCLO                      1.00000E-20   0.00000E+00   2.84935E-45   -44.5453
 CRO4-2                    1.00000E-20   0.00000E+00   1.26903E-34   -33.8965
 HCLO2                     1.00000E-20   0.00000E+00   1.02675E-87   -86.9885
 HCRO4-1                   1.00000E-20   0.00000E+00   3.83517E-35   -34.4162
 CR2O7-2                   1.00000E-20   0.00000E+00   5.34416E-68   -67.2721
 HO2-1                     1.00000E-20   0.00000E+00   7.10153E-51   -50.1486
 CR+2                      1.00000E-20   0.00000E+00   2.20654E-23   -22.6563
 CO1H2O2                   1.00000E-20   0.00000E+00   2.7988E-105  -104.5530
 CO+3                      1.00000E-20   0.00000E+00   3.73219E-42   -41.4280
 O2                        1.00000E-20   0.00000E+00   2.17223E-58   -57.6631
 CLO4-1                    1.00000E-20   0.00000E+00   5.5717E-133  -132.2540
 CLO3-1                    1.00000E-20   0.00000E+00   1.0705E-105  -104.9704
 CLO2-1                    1.00000E-20   0.00000E+00   1.07460E-82   -81.9688
 CLO2                      1.00000E-20   0.00000E+00   1.1652E-100   -99.9336
 CLO-1                     1.00000E-20   0.00000E+00   6.17706E-46   -45.2092
 CL2                       1.00000E-20   0.00000E+00   4.04170E-50   -49.3934
 Solution Properties:   pH =   7.0000    Eh =   -0.0000 V     I =   0.0856
                        pe =  -0.0000    Ah =   -0.0000 kJ   m* =   0.1712
                        Aw =   0.9966    Os =    1.1033     pKw =  13.9973
                        At1= 1.0000E-20  At2= 1.2744E-07 (equiv_mol/kg_H2O)

 HEMATITE                     Status ENTERED     Driving force  0.0000E+00
 Moles 3.3409E-02, Mass 1.0670E+00, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.20000E+00  NI   0.00000E+00  NA   0.00000E+00
 H2O  6.00000E-01  CR   0.00000E+00  CO   0.00000E+00
 FE   4.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00

 NIFE2O4                      Status ENTERED     Driving force  0.0000E+00
 Moles 5.8715E-03, Mass 1.9660E-01, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.14286E+00  NI   1.42857E-01  NA   0.00000E+00
 H2O  5.71429E-01  CR   0.00000E+00  CO   0.00000E+00
 FE   2.85714E-01  CL   0.00000E+00  H+1 -1.14286E+00

 CR2O3                        Status ENTERED     Driving force  0.0000E+00
 Moles 3.9597E-03, Mass 1.2037E-01, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.20000E+00  NI   0.00000E+00  NA   0.00000E+00
 H2O  6.00000E-01  FE   0.00000E+00  CO   0.00000E+00
 CR   4.00000E-01  CL   0.00000E+00  H+1 -1.20000E+00

 COCR2O4                      Status ENTERED     Driving force  0.0000E+00
 Moles 1.1877E-03, Mass 3.8504E-02, Volume fraction 0.0000E+00  Mole fractions:
 ZE   1.14286E+00  CO   1.42857E-01  NA   0.00000E+00
 H2O  5.71429E-01  NI   0.00000E+00  FE   0.00000E+00
 CR   2.85714E-01  CL   0.00000E+00  H+1 -1.14286E+00
POLY: l-st p
   ... the command in full is LIST_STATUS
 *** STATUS FOR ALL PHASES
 PHASE                    STATUS    DRIVING FORCE   MOLES
 NIFE2O4                  ENTERED      0.000000E+00    5.871536E-03
 HEMATITE                 ENTERED      0.000000E+00    3.340878E-02
 CR2O3                    ENTERED      0.000000E+00    3.959678E-03
 COCR2O4                  ENTERED      0.000000E+00    1.187738E-03
 AQUEOUS                  ENTERED      0.000000E+00    5.565313E+01
 FECR2O4                  ENTERED     -1.007600E-01    0.000000E+00
 FE2O2O2H2                ENTERED     -1.872978E-01    0.000000E+00
 FEOOH                    ENTERED     -2.260402E-01    0.000000E+00
 COFE2O4                  ENTERED     -8.149192E-01    0.000000E+00
 FEO3H3                   ENTERED     -1.157510E+00    0.000000E+00
 NICR2O4                  ENTERED     -1.415362E+00    0.000000E+00
 FE2O3_GAMMA              ENTERED     -1.461433E+00    0.000000E+00
 MAGNETITE                ENTERED     -1.556302E+00    0.000000E+00
 NIO2H2                   ENTERED     -3.146330E+00    0.000000E+00
 NIO                      ENTERED     -4.159999E+00    0.000000E+00
 ENTERED PHASES WITH DRIVING FORCE LESS THAN   -4.169527E+00
 NIO_S2 HALITE COO2H2 FEO2H2 NA2CR2O4 NA2FEO2 CO3O4 WUSTITE COO CRO2 NA2CRO4
 NA2CRO4_S2 NIOOH CR5O12 NAOH NAOH_S2 CR8O21 CRO3 GAS NA2O2 NA2O2_S2 NA2O
 NA2O_S2 NA2O_S3 NAO2 FCC_A1 BCC_A2
 SUSPENDED PHASES:
 REF_ELECTRODE
POLY: sh b n n(*)
   ... the command in full is SHOW_VALUE
 B=1005.9467
 N=55.697555
 N(H2O)=55.508435, N(H+1)=-5.2909903E-2, N(ZE)=5.2936192E-2, N(NA)=8.5554E-2,
    N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
    N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY:
POLY: @@ Save the workspace for the single-point equilibrium
POLY: @@ of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY:
POLY: save TCEX53_c.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continuePOLY:
POLY: @@ ==========================================================
POLY: @@ Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl
POLY: @@ ==========================================================
POLY:
POLY: @@ Define the mapping variables for Pourbaix diagram:
POLY: @@                          pH from  0   to 14
POLY: @@                          Eh from -1.2 to 1.5 (V)
POLY: s-a-v 1 lnacr(H+1) -32.22994 0 0.5
   ... the command in full is SET_AXIS_VARIABLE
POLY: s-a-v 2 mur(Ze) -150000 200000 5000
   ... the command in full is SET_AXIS_VARIABLE
POLY: 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:
POLY: @@ Add the starting points as initial equilibria:
POLY: @@ These may be enforced in 2 or 4 directions with
POLY: @@ the option >
POLY:
POLY: add 1>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM

POLY: add -1>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add 2>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: add -2>
   ... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY: @@ You can have more starting points at other pH-Eh
POLY: @@ conditions [corresponding to varied lnacr(H+1)
POLY: @@ and mur(Ze) values], and add them as initial equilibria.
POLY: @@ s-c lnacr(H+1)=-23.0
POLY: @@ s-c mur(ZE)=-2000
POLY: @@ l-c
POLY: @@ c-e
POLY: @@ l-e ,x
POLY:
POLY: li-in-eq
   ... the command in full is LIST_INITIAL_EQUILIBRIA
 No 1  +1> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
    N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
 No 2  -1> P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
    N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
 No 3  +2> P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
    N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
 No 4  -2> P=100000, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
    N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
    N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
POLY:
POLY: @@ Save the workspace for the Pourbaix diagram settings
POLY: @@ of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY: save TCEX53_d.POLY3 y
   ... the command in full is SAVE_WORKSPACES
POLY:Hit RETURN to continuePOLY:
POLY: @@ Perform the mapping calculation:
POLY: @@ ---------------------------------------------------------
POLY: @@ Due to the complexity of the aqueous solution model (SIT),
POLY: @@ a complete mapping calculation of the Pourbaix diagram
POLY: @@ may take a long time. Be patient...
POLY: @@ ---------------------------------------------------------
POLY: MAP
 Version S mapping is selected

 Organizing start points

Using ADDED start equilibria


 Tie-lines not in the plane of calculation
 Generating start point   1
 Generating start point   2
 Generating start point   3
 Generating start point   4
 Generating start point   5
 Generating start point   6
 Generating start point   7
 Generating start point   8
 Generating start point   9
 Generating start point  10
 Working hard
 Generating start point  11
 Generating start point  12

 Phase region boundary   1 at:  -1.541E+01 -4.404E-12
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated..                      35 equilibria
 Terminating at axis limit.

 Phase region boundary   2 at:  -3.223E+01 -4.165E+04
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated.                       38 equilibria

 Phase region boundary   3 at:  -1.404E+01  3.415E+03
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
  ** NIFE2O4

 Phase region boundary   4 at:  -1.404E+01  3.415E+03
     AQUEOUS
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
 Calculated.                        7 equilibria

 Phase region boundary   5 at:  -1.110E+01  1.070E+04
     AQUEOUS
  ** COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
```

```
Phase region boundary   6 at:  -1.110E+01  1.070E+04
    AQUEOUS
    CR2O3
 ** FECR2O4
    HEMATITE
Calculated.                      8 equilibria

Phase region boundary   7 at:  -7.729E+00  1.905E+04
    AQUEOUS
    CR2O3
 ** FECR2O4
 ** HEMATITE

Phase region boundary   8 at:  -7.729E+00  1.905E+04
    AQUEOUS
    CR2O3
 ** FECR2O4
Calculated.                      9 equilibria

Phase region boundary   9 at:  -7.729E+00 -1.955E+04
 ** GAS
    AQUEOUS
    CR2O3
 ** FECR2O4

Phase region boundary  10 at:  -7.729E+00 -1.955E+04
    GAS
    AQUEOUS
    CR2O3
 ** FECR2O4
Calculated.                      5 equilibria

Phase region boundary  11 at:  -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
 ** CR2O3
 ** FECR2O4

Phase region boundary  12 at:  -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
 ** FECR2O4
Calculated                      44 equilibria

Phase region boundary  13 at:  -7.169E+00 -1.817E+04
    GAS
    AQUEOUS
 ** CR2O3
Calculated.                      2 equilibria

Phase region boundary  14 at:  -7.259E+00 -1.839E+04
 ** GAS
    AQUEOUS
 ** CR2O3

Phase region boundary  15 at:  -7.259E+00 -1.839E+04
    AQUEOUS
 ** CR2O3
Calculated.                     10 equilibria

Phase region boundary  16 at:  -7.259E+00  2.259E+04
    AQUEOUS
 ** CR2O3
 ** HEMATITE

Phase region boundary  17 at:  -7.259E+00  2.259E+04
    AQUEOUS
 ** CR2O3
    HEMATITE
Calculated.                     32 equilibria

Phase region boundary  18 at:  -1.110E+01  7.654E+04
    AQUEOUS
 ** COCR2O4
 ** CR2O3
    HEMATITE

Phase region boundary  19 at:  -1.110E+01  7.654E+04
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
Calculated.                      7 equilibria

Phase region boundary  20 at:  -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
 ** NIFE2O4

Phase region boundary  21 at:  -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
    NIFE2O4
Calculated..                     38 equilibria
Terminating at axis limit.

Phase region boundary  22 at:  -1.404E+01  6.628E+04
    AQUEOUS
    COCR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                      1 equilibria

Phase region boundary  23 at:  -1.404E+01  6.733E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
 ** NIFE2O4

Phase region boundary  24 at:  -1.404E+01  6.733E+04
    AQUEOUS
```

```
    CO3O4
    COCR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                      2 equilibria

Phase region boundary  25 at:  -1.404E+01  6.745E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
    HEMATITE
 ** NIFE2O4

Phase region boundary  26 at:  -1.404E+01  6.745E+04
    AQUEOUS
    CO3O4
    HEMATITE
 ** NIFE2O4
Calculated.                      5 equilibria

Phase region boundary  27 at:  -1.404E+01  8.332E+04
 ** GAS
    AQUEOUS
    CO3O4
    HEMATITE
 ** NIFE2O4

Phase region boundary  28 at:  -1.404E+01  8.332E+04
    GAS
    AQUEOUS
    CO3O4
    HEMATITE
 ** NIFE2O4
Calculated.                     11 equilibria

Phase region boundary  29 at:  -1.257E+01  8.794E+04
    GAS
    AQUEOUS
    CO3O4
 ** HALITE
    HEMATITE
 ** NIFE2O4

Phase region boundary  30 at:  -1.257E+01  8.794E+04
    GAS
    AQUEOUS
    CO3O4
    HALITE
    HEMATITE
 ** NIFE2O4
Calculated                     33 equilibria

Phase region boundary  31 at:  -1.257E+01  8.794E+04
    GAS
    AQUEOUS
    CO3O4
 ** HALITE
    HEMATITE
Calculated.                      9 equilibria

Phase region boundary  32 at:  -8.749E+00  9.740E+04
    GAS
    AQUEOUS
 ** CO3O4
 ** HALITE
    HEMATITE

Phase region boundary  33 at:  -8.749E+00  9.740E+04
    GAS
    AQUEOUS
 ** HALITE
    HEMATITE
Calculated.                     18 equilibria

Phase region boundary  34 at:  -1.463E+00  1.159E+05
    GAS
    AQUEOUS
 ** HALITE
 ** HEMATITE

Phase region boundary  35 at:  -1.463E+00  1.159E+05
    GAS
    AQUEOUS
 ** HALITE
Calculated                     48 equilibria

Phase region boundary  36 at:  -1.463E+00  1.159E+05
    GAS
    AQUEOUS
 ** HEMATITE
Calculated                      5 equilibria

Phase region boundary  37 at:  -1.463E+00  1.159E+05
    GAS
    AQUEOUS
    HALITE
 ** HEMATITE
Calculated                     27 equilibria

Phase region boundary  38 at:  -8.749E+00  9.740E+04
    GAS
    AQUEOUS
 ** CO3O4
    HEMATITE
Calculated.                      8 equilibria

Phase region boundary  39 at:  -1.021E+01  9.281E+04
 ** GAS
    AQUEOUS
 ** CO3O4
    HEMATITE

Phase region boundary  40 at:  -1.021E+01  9.281E+04
    AQUEOUS
 ** CO3O4
    HEMATITE
```

```
Calculated.                      5 equilibria

Phase region boundary  41 at:  -1.211E+01  7.398E+04
    AQUEOUS
 ** CO3O4
 ** COCR2O4
    HEMATITE

Phase region boundary  42 at:  -1.211E+01  7.398E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary  43 at:  -1.211E+01  7.398E+04
    AQUEOUS
 ** COCR2O4
    HEMATITE
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary  44 at:  -1.211E+01  7.398E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
    HEMATITE
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary  45 at:  -1.021E+01  9.281E+04
 ** GAS
    AQUEOUS
    HEMATITE
Calculated.                     20 equilibria

Phase region boundary  46 at:  -1.208E+00  1.151E+05
 ** GAS
    AQUEOUS
 ** HEMATITE

Phase region boundary  47 at:  -1.208E+00  1.151E+05
 ** GAS
    AQUEOUS
Calculated..                      4 equilibria
Terminating at axis limit.

Phase region boundary  48 at:  -1.208E+00  1.151E+05
    AQUEOUS
 ** HEMATITE
Calculated.                     28 equilibria
Terminating at known equilibrium

Phase region boundary  49 at:  -1.208E+00  1.151E+05
    GAS
    AQUEOUS
 ** HEMATITE
Calculated                     14 equilibria

Phase region boundary  50 at:  -1.021E+01  9.281E+04
 ** GAS
    AQUEOUS
    CO3O4
    HEMATITE
Calculated.                      9 equilibria
Terminating at known equilibrium

Phase region boundary  51 at:  -8.749E+00  9.740E+04
    GAS
    AQUEOUS
 ** CO3O4
    HALITE
    HEMATITE
Calculated                     39 equilibria

Phase region boundary  52 at:  -1.257E+01  8.794E+04
    GAS
    AQUEOUS
    CO3O4
 ** HALITE
    HEMATITE
    NIFE2O4
Calculated..                     41 equilibria
Terminating at axis limit.

Phase region boundary  53 at:  -1.404E+01  8.332E+04
 ** GAS
    AQUEOUS
    CO3O4
    HEMATITE
    NIFE2O4
Calculated..                     38 equilibria
Terminating at axis limit.

Phase region boundary  54 at:  -1.404E+01  6.745E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
    HEMATITE
    NIFE2O4
Calculated.                     27 equilibria

Phase region boundary  55 at:  -2.249E+01  3.456E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
 ** COFE2O4
    HEMATITE
    NIFE2O4

Phase region boundary  56 at:  -2.249E+01  3.456E+04
    AQUEOUS
    CO3O4
 ** COCR2O4
    COFE2O4
```

```
     HEMATITE
     NIFE2O4
++++++
```

```
 ** CR2O3
    FECR2O4
 ** HEMATITE

Phase region boundary  72 at:  -7.752E+00  1.899E+04
    AQUEOUS
 ** CR2O3
    FECR2O4
    HEMATITE
Calculated.                      8 equilibria
Terminating at known equilibrium

Phase region boundary  73 at:  -7.752E+00  1.899E+04
    AQUEOUS
    FECR2O4
 ** HEMATITE
Calculated.                     16 equilibria

Phase region boundary  74 at:  -1.286E+01 -1.893E+04
    AQUEOUS
    FECR2O4
 ** HEMATITE
 ** MAGNETITE

Phase region boundary  75 at:  -1.286E+01 -1.893E+04
    AQUEOUS
    FECR2O4
 ** HEMATITE
    MAGNETITE
Calculated.                      4 equilibria

Phase region boundary  76 at:  -1.395E+01 -2.164E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
 ** HEMATITE
    MAGNETITE

Phase region boundary  77 at:  -1.395E+01 -2.164E+04
    AQUEOUS
    COFE2O4
    FECR2O4
 ** HEMATITE
    MAGNETITE
Calculated.                      2 equilibria

Phase region boundary  78 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
 ** HEMATITE
    MAGNETITE
 ** NIFE2O4

Phase region boundary  79 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
 ** HEMATITE
    MAGNETITE
    NIFE2O4
Calculated..                    38 equilibria
Terminating at axis limit.

Phase region boundary  80 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    MAGNETITE
 ** NIFE2O4
Calculated.                      5 equilibria

Phase region boundary  81 at:  -1.555E+01 -3.682E+04
    AQUEOUS
 ** BCC_A2
    COFE2O4
    FECR2O4
    MAGNETITE
 ** NIFE2O4

Phase region boundary  82 at:  -1.555E+01 -3.682E+04
    AQUEOUS
    BCC_A2
    COFE2O4
    FECR2O4
    MAGNETITE
 ** NIFE2O4
Calculated..                    35 equilibria
Terminating at axis limit.

Phase region boundary  83 at:  -1.555E+01 -3.682E+04
    AQUEOUS
 ** BCC_A2
    COFE2O4
    FECR2O4
    MAGNETITE
Calculated.                      2 equilibria

Phase region boundary  84 at:  -1.548E+01 -3.681E+04
    AQUEOUS
 ** BCC_A2
 ** COFE2O4
    FECR2O4
    MAGNETITE

Phase region boundary  85 at:  -1.548E+01 -3.681E+04
    AQUEOUS
 ** BCC_A2
    FECR2O4
    MAGNETITE
Calculated.                      4 equilibria

Phase region boundary  86 at:  -1.473E+01 -3.690E+04
 ** GAS
    AQUEOUS
 ** BCC_A2
```

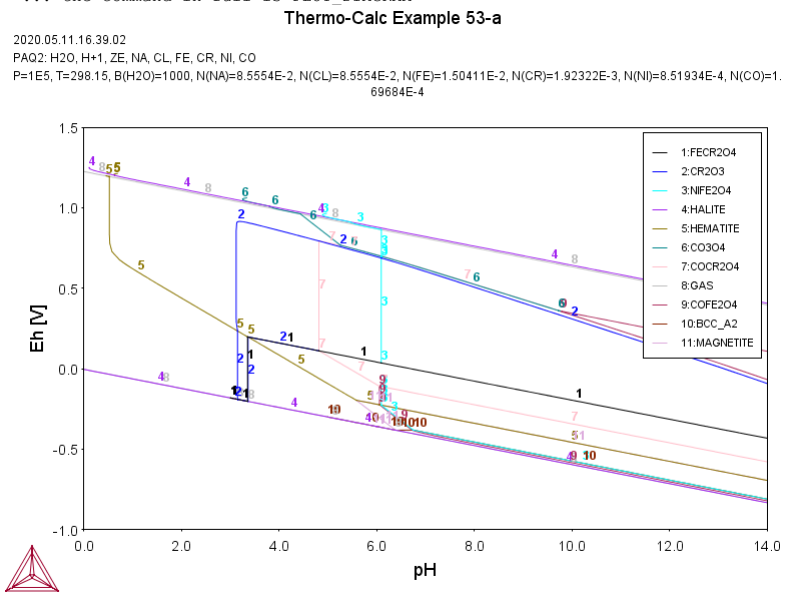
```
    FECR2O4
    MAGNETITE

Phase region boundary  87 at:  -1.473E+01 -3.690E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
    MAGNETITE
Calculated.                      5 equilibria

Phase region boundary  88 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
 ** MAGNETITE

Phase region boundary  89 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
Calculated.                      8 equilibria

Phase region boundary  90 at:  -1.280E+01 -3.214E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
 ** HALITE

Phase region boundary  91 at:  -1.280E+01 -3.214E+04
    GAS
    AQUEOUS
 ** BCC_A2
    FECR2O4
    HALITE
Calculated                     201 equilibria

Phase region boundary  92 at:  -1.280E+01 -3.214E+04
    GAS
    AQUEOUS
    FECR2O4
 ** HALITE
Calculated.                     14 equilibria

Phase region boundary  93 at:  -7.005E+00 -1.778E+04
    GAS
    AQUEOUS
 ** FECR2O4
 ** HALITE

Phase region boundary  94 at:  -7.005E+00 -1.778E+04
    GAS
    AQUEOUS
 ** HALITE
Calculated..                     16 equilibria
Terminating at axis limit.

Phase region boundary  95 at:  -7.005E+00 -1.778E+04
    GAS
    AQUEOUS
 ** FECR2O4
                                                  +                                                  ++

Phase region boundary  96 at:  -7.005E+00 -1.778E+04
    GAS
    AQUEOUS
 ** FECR2O4
    HALITE
Calculated                      23 equilibria

Phase region boundary  97 at:  -1.280E+01 -3.214E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** HALITE
Calculated.                      6 equilibria

Phase region boundary  98 at:  -1.381E+01 -3.464E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** HALITE
 ** MAGNETITE

Phase region boundary  99 at:  -1.381E+01 -3.464E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** HALITE
    MAGNETITE
Calculated..                     38 equilibria
Terminating at axis limit.

Phase region boundary 100 at:  -1.381E+01 -3.464E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** MAGNETITE
                                                  +                                                  ++

Phase region boundary 101 at:  -1.381E+01 -3.464E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
    HALITE
 ** MAGNETITE
Calculated                      61 equilibria
```

```
Phase region boundary 102 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
    FECR2O4
 ** MAGNETITE
Calculated.                      3 equilibria

Phase region boundary 103 at:  -1.472E+01 -3.688E+04
 ** GAS
    AQUEOUS
    FECR2O4
 ** MAGNETITE

Phase region boundary 104 at:  -1.472E+01 -3.688E+04
    AQUEOUS
    FECR2O4
 ** MAGNETITE
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary 105 at:  -1.472E+01 -3.688E+04
 ** GAS
    AQUEOUS
    FECR2O4
Calculated.                     15 equilibria
Terminating at known equilibrium

Phase region boundary 106 at:  -1.472E+01 -3.688E+04
 ** GAS
    AQUEOUS
    FECR2O4
    MAGNETITE
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary 107 at:  -1.390E+01 -3.486E+04
    GAS
    AQUEOUS
    BCC_A2
    FECR2O4
 ** MAGNETITE
Calculated                      46 equilibria

Phase region boundary 108 at:  -1.473E+01 -3.690E+04
 ** GAS
    AQUEOUS
    BCC_A2
    FECR2O4
    MAGNETITE
Calculated..                     38 equilibria
Terminating at axis limit.

Phase region boundary 109 at:  -1.548E+01 -3.681E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
    MAGNETITE
Calculated.                      5 equilibria
Terminating at known equilibrium

Phase region boundary 110 at:  -1.548E+01 -3.681E+04
    AQUEOUS
    BCC_A2
 ** COFE2O4
    FECR2O4
    MAGNETITE
Calculated..                     37 equilibria
Terminating at axis limit.

Phase region boundary 111 at:  -1.555E+01 -3.682E+04
    AQUEOUS
 ** BCC_A2
    COFE2O4
    FECR2O4
    MAGNETITE
    NIFE2O4
Calculated..                     35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 112 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
    MAGNETITE
 ** NIFE2O4
Calculated.                      1 equilibria

Phase region boundary 113 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
 ** MAGNETITE
 ** NIFE2O4

Phase region boundary 114 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                      4 equilibria

Phase region boundary 115 at:  -1.404E+01 -1.073E+04
    AQUEOUS
 ** COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
 ** NIFE2O4

Phase region boundary 116 at:  -1.404E+01 -1.073E+04
    AQUEOUS
    COCR2O4
```

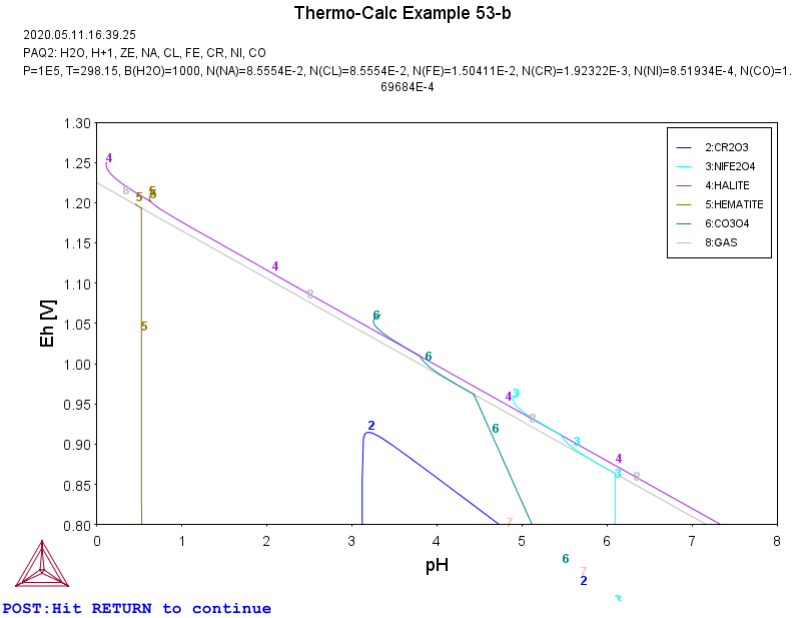
```
    COFE2O4
    FECR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                      1 equilibria
Terminating at known equilibrium

Phase region boundary 117 at:  -1.404E+01 -1.073E+04
    AQUEOUS
 ** COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
Calculated.                      2 equilibria

Phase region boundary 118 at:  -1.395E+01 -1.051E+04
    AQUEOUS
 ** COCR2O4
 ** COFE2O4
    FECR2O4
    HEMATITE

Phase region boundary 119 at:  -1.395E+01 -1.051E+04
    AQUEOUS
 ** COCR2O4
    FECR2O4
    HEMATITE
Calculated.                      7 equilibria
Terminating at known equilibrium

Phase region boundary 120 at:  -1.395E+01 -1.051E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
    HEMATITE
Calculated.                      3 equilibria

Phase region boundary 121 at:  -1.395E+01 -2.164E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
    HEMATITE
 ** MAGNETITE

Phase region boundary 122 at:  -1.395E+01 -2.164E+04
    AQUEOUS
 ** COFE2O4
    FECR2O4
    HEMATITE
    MAGNETITE
Calculated.                      1 equilibria
Terminating at known equilibrium

Phase region boundary 123 at:  -1.395E+01 -2.164E+04
    AQUEOUS
    FECR2O4
    HEMATITE
 ** MAGNETITE
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary 124 at:  -1.395E+01 -2.164E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
 ** MAGNETITE
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary 125 at:  -1.395E+01 -1.051E+04
    AQUEOUS
    COCR2O4
 ** COFE2O4
    FECR2O4
    HEMATITE
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary 126 at:  -1.404E+01 -1.073E+04
    AQUEOUS
 ** COCR2O4
    COFE2O4
    FECR2O4
    HEMATITE
    NIFE2O4
Calculated..                     38 equilibria
Terminating at axis limit.

Phase region boundary 127 at:  -1.404E+01 -2.186E+04
    AQUEOUS
    COFE2O4
    FECR2O4
    HEMATITE
 ** MAGNETITE
    NIFE2O4
Calculated..                     38 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 128 at:  -7.752E+00  1.899E+04
    AQUEOUS
    CR2O3
    FECR2O4
 ** HEMATITE
Calculated.                      2 equilibria
Terminating at known equilibrium

Phase region boundary 129 at:  -7.752E+00 -1.961E+04
 ** GAS
    AQUEOUS
    CR2O3
    FECR2O4
Calculated.                      2 equilibria
Terminating at known equilibrium
```

```
Phase region boundary 130 at:  -1.110E+01  1.070E+04
    AQUEOUS
 ** COCR2O4
    CR2O3
    FECR2O4
    HEMATITE
Calculated.                      1 equilibria
Terminating at known equilibrium

Phase region boundary 131 at:  -1.404E+01  3.415E+03
    AQUEOUS
    COCR2O4
    CR2O3
    FECR2O4
    HEMATITE
 ** NIFE2O4
Calculated.                      1 equilibria
Terminating at known equilibrium

Phase region boundary 132 at:  -1.541E+01 -4.404E-12
    AQUEOUS
    COCR2O4
    CR2O3
 ** FECR2O4
    HEMATITE
    NIFE2O4
Calculated.                      4 equilibria
Terminating at known equilibrium

Phase region boundary 133 at:  -3.020E+01 -4.404E-12
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
    NIFE2O4
Calculated..                      9 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 134 at:  -3.020E+01 -4.404E-12
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
    NIFE2O4
Calculated.                     54 equilibria
Terminating at known equilibrium

Phase region boundary 135 at:  -1.610E+01  5.964E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.                     21 equilibria
Terminating at known equilibrium

Phase region boundary 136 at:  -1.610E+01  5.964E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.                      7 equilibria
Terminating at known equilibrium

Phase region boundary 137 at:  -1.612E+01  5.959E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.                     14 equilibria
Terminating at known equilibrium

Phase region boundary 138 at:  -1.612E+01  5.959E+04
    AQUEOUS
 ** CO3O4
    COCR2O4
    HEMATITE
    NIFE2O4
Calculated.                      6 equilibria
Terminating at known equilibrium

Phase region boundary 139 at:  -1.612E+01  5.825E+04
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
    NIFE2O4
Calculated..                     34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 140 at:  -1.612E+01  5.825E+04
    AQUEOUS
    COCR2O4
 ** CR2O3
    HEMATITE
    NIFE2O4
Calculated.                      6 equilibria
Terminating at known equilibrium

Phase region boundary 141 at:  -1.612E+01 -1.748E+03
    AQUEOUS
    COCR2O4
    CR2O3
 ** FECR2O4
    HEMATITE
    NIFE2O4
Calculated..                     34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 142 at:  -1.612E+01 -1.748E+03
    AQUEOUS
```

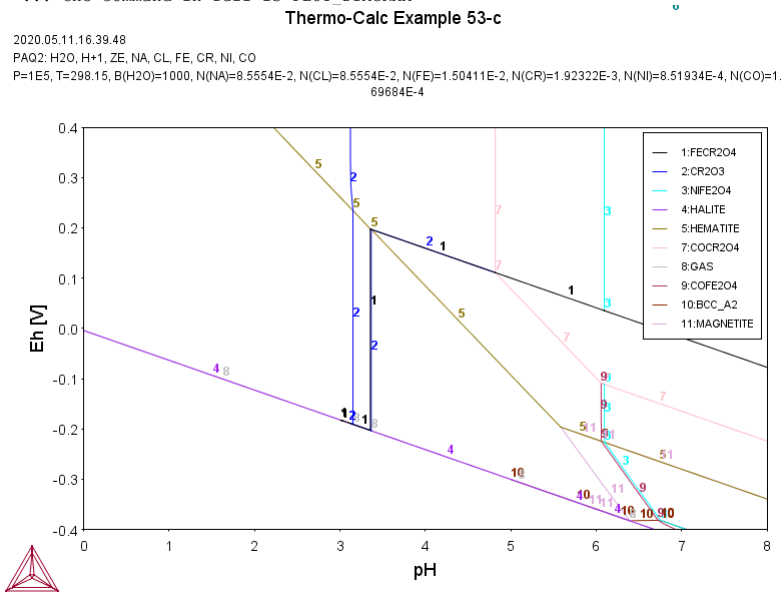
```
     COCR2O4
     CR2O3
  ** FECR2O4
     HEMATITE
     NIFE2O4
 Calculated.                        6 equilibria
 Terminating at known equilibrium
 *** BUFFER SAVED ON FILE: c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex53\TCEX53_d.POLY3
 CPU time for mapping                    1015 seconds
POLY:
POLY: @@ Plot the calculated Pourbaix diagram (and others):
POLY: @@ ----------------------------------------------------------
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2

 Setting automatic diagram axes

POST: l-sym
   ... the command in full is LIST_SYMBOLS
 DEFINED CONSTANTS
    AH2O=55.508435, RNF=96485.309, ZERO=0
 DEFINED FUNCTIONS AND VARIABLES%
    EH=MUR(ZE)/RNF
    PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
    TEMP_C=T-273.15
POST:Hit RETURN to 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:
POST: s-d-a y Eh
   ... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text y n Eh [V]
   ... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-t-m-s y
   ... the command in full is SET_TRUE_MANUAL_SCALING
 COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: s-l-c e
   ... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: s-s-s x n 0 14
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n -1.0 1.5
   ... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-a
   ... the command in full is SET_TITLE
POST: pl,,,
   ... the command in full is PLOT_DIAGRAM
```




```
POST: make TCEX53.EXP y
   ... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:Hit RETURN to continue
POST:
POST: s-s-s x n 0 8
   ... the command in full is SET_SCALING_STATUS
POST: s-s-s y n .8 1.3
   ... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-b
   ... the command in full is SET_TITLE
POST:
POST: pl,,,
   ... the command in full is PLOT_DIAGRAM
```




```
POST:Hit RETURN to continue
POST:
POST: s-s-s y n -.4 .4
   ... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-c
   ... the command in full is SET_TITLE
POST:
POST: pl,,,
   ... the command in full is PLOT_DIAGRAM
```




```
POST:Hit RETURN to continue
POST:
POST:
POST: @@ ----------------------------------------------------------
POST: @@ From the same mapping calculations, you can plot more
POST: @@ diagrams, using different X-Y axis variables (for such
POST: @@ purposes, it is convenient to use pre-defined symbols as
POST: @@ listed at the end of this macro file).
POST: @@ ----------------------------------------------------------
POST:
POST: SET-INTERACTIVE
   ... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex54

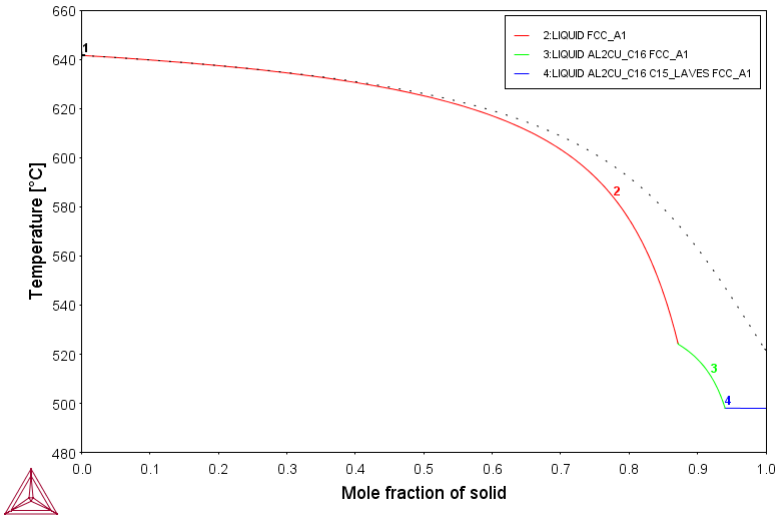
```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex54\tcex54.TCM.test"
SYS: SET_ECHO
SYS:
SYS: @@ Simulating the soldification of a Al-2.1Cu-1Si alloy
SYS: @@ with a Scheil calculation including back diffusion
SYS:
SYS: @@ This is an example of a solidification simulation
SYS: @@ of a Al-2.1Cu-1Si alloy. The back diffusion option
SYS: @@ in the Scheil module is used, i.e. there is back
SYS: @@ diffusion in the primary phase.
SYS:
SYS: SET-GES-VERSION 6
SYS: GO SCHEIL
SCHEIL: USE-BACK-DIFFUSION YES
SCHEIL: START-WIZARD
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
Database /TCFE10/: ALDEMO
 Current database: Aluminum Demo Database v4.0

 VA                      /-  DEFINED
Major element or alloy: AL
Composition input in mass (weight) percent? /Y/: N
 Composition will be taken to be in mole percent
1st alloying element: CU
Mole percent /1/: 2.1
2nd alloying element: SI
Mole percent /1/: 1.0
Next alloying element:
Temperature (C) /2000/: 1000
 VA                      /-  DEFINED
 REINITIATING GES .....
 AL  DEFINED
 CU  DEFINED
 SI  DEFINED


 This database has following phases for the defined system

 LIQUID:L                AL2CU_C16               ALCU_DEL
 ALCU_EPS                ALCU_ETA                ALCU_ZETA
 ALZR2_B82               BCC_A2                  BCC_B2
 C14_LAVES               C15_LAVES               C36_LAVES
 CU15SI4_EPSILON         CU33SI7_DELTA           CU56SI11_GAMMA
 CUSI_ETA                DIAMOND_A4              FCC_A1
 GAMMA_D83               GAMMA_H                 HCP_A3
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

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

    The following phases are retained in this system:

 LIQUID:L                AL2CU_C16               ALCU_DEL
 ALCU_EPS                ALCU_ETA                ALCU_ZETA
 ALZR2_B82               BCC_A2                  BCC_B2
 C14_LAVES               C15_LAVES               C36_LAVES
 CU15SI4_EPSILON         CU33SI7_DELTA           CU56SI11_GAMMA
 CUSI_ETA                DIAMOND_A4              FCC_A1
 GAMMA_D83               GAMMA_H                 HCP_A3

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

OK? /Y/: Y
 *** ERROR GAS INPUT IGNORED
16:41:28,547 INFO  *** Invoking Gibbs Energy System v6 ***
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, Calphad,15 317-425 (1991)'
  'Volume data from TCFE4, 2006'
  'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
      thermal conductivity'
  'M J Assael, High Temp High Press 41 (2012); Sb, Pb, Bi, Ni, Ag'
  'M Ghasemi, Thermo-Calc Software AB (2020)'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
  'M J Assael, J Phys Chem Ref Data 41 (2012) 033101; Cd, Co, Ga, In, Hg, Si,
       Tl, Zn'
  'I. Ansara (Editor), COST 507, (1998)'
  'M Ghasemi, Thermo-Calc Software AB (2019)'
  'C.-Y. He,Calphad, 33,200-210 (2009),Al-Cu-Si'
  'J. Groebner,Calphad,20(2)247-254(1996),Al-C-Si'
  'X.Y. Yan,J. Alloy and Compd. 308, 221-229 (2000),CU-Si'
  'L. Kjellqvist, Thermo-Calc Software AB, Stockholm, 2010; Unassessed
      parameter, linear combination of unary volume data'
  'H-L Chen, in TCAL3.0, Assessment, extrapolation and assumption'
```

```
  'Hai-Lin Chen, electrical resistivity
       thermal conductivity (2020)'
  'L. Kjellqvist, Thermo-Calc Software AB, Sweden 2012; Molar volumes'
  'H-L Chen, Evaluation of molar volume'
  'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
  'N. Dupin, Calphad, 25(2)279-298(2001),Al-Cr-Ni'
  'Nathalie Dupin, in TCNI6.0, Refinement of Al-Ni'
  'Volume data, N. Dupin 2008'
  'H-L Chen, in TCAL2.0, Assessment, extrapolation and assumption'
  'J.R.Zhao, Y.Du, to be submitted, 2010,Sn-Sr,Cu-Mg-Si'
  'W.H. Sun, unpublished (2010),Cu-Si-Zn,Cu-Ni-Zn'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'H-L Chen, in TCAL1.2, assessment of Al-Cu-Mg-Si'
 -OK-
Should any phase have a miscibility gap check? /N/: N
Mobility Database /MALDEMO/: MALDEMO
 Current database: Al-Alloys Mobility demo database v2.0

 VA                      /-  DEFINED
 AL  DEFINED
 CU  DEFINED
 SI  DEFINED


 This database has following phases for the defined system

 LIQUID:L                 FCC_A1
Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

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

    The following phases are retained in this system:

 LIQUID:L                 FCC_A1

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

OK? /Y/: Y
 *** ERROR GAS INPUT IGNORED
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'This parameter has not been assessed'
  'Lijun Zhang, Yong Du et al.,"Atomic mobilities and diffusivities in the
      fcc, L12 and B2 phases of the Ni-Al system",2010'
  'G. Ghosh, Acta Mater.,2001,49,2609-2624'
  'D.D. Liu,L.J. Zhang et al. "The assessment of atomic mobilities of Al and
      Cu in fcc Al-Cu alloys",CALPHAD,2009,33,761-768'
  'D.D. Liu, L.J. Zhang et al., "The assessment of atomic mobilities of Al,
      Cu and Si in fcc Al-Cu-Si system",2010'
  'L. Zhang et al., Acta Mater., 58(2010)3664.'
  'Y. Du et al., Mat. Sci. Eng. A363(2003)140.'
 INFO: Forcing option USE_POLY3 for complex phase ALZR2_B82
 INFO: Forcing option USE_POLY3 for complex phase BCC_A2
 -OK-
Should any phase have a miscibility gap check? /N/: N
  LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/: NONE
Temperature time dependence /LINEAR/: LINEAR
Cooling rate (K/s) /1/: 1.0
Expression for secondary dendrite arm spacing /CONSTANT/: POWER_LAW
 Power law in the form c*(cooling rate)^-n
Exponent n /.33/: 5.0E-5
Scaling factor c /5E-05/: 0.33
Primary phase /AUTOMATIC/: AUTOMATIC
 This command is a combination of CHANGE_STATUS and SET_CONDITION
 to calculate directly when a phase may form by releasing one condition.
 You must release one of these conditions
 T=1273.15, X(CU)=2.1E-2, X(SI)=1E-2, P=1E5, N=1    DEGREES OF FREEDOM 0
 PHASE CHANGE AT 914.742752934
FCC_A1#1 forms
 Testing POLY result by global minimization procedure
Calculated         17676 grid points in             0 s
  CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
...OK

 Phase Region from    914.833     for:
     LIQUID
 Terminating at    914.933
 Calculated     4 equilibria

 Phase Region from    914.833     for:
     LIQUID
 Global check of adding phase at  9.14743E+02
 Calculated     3 equilibria

 Phase Region from    914.743     for:
     LIQUID
     FCC_A1
 Global test at  9.06833E+02 .... OK
 Global test at  8.96833E+02 .... OK
 Global test at  8.86833E+02 .... OK
 Global test at  8.76833E+02 .... OK
 Global test at  8.66833E+02 .... OK
 Global test at  8.56833E+02 .... OK
 Global test at  8.46833E+02 .... OK
 Global test at  8.36833E+02 .... OK
 Global test at  8.26833E+02 .... OK
 Global test at  8.16833E+02 .... OK
 Global test at  8.06833E+02 .... OK
 Global test at  7.96833E+02 .... OK
 Global check of removing phase at  7.94498E+02
 Backtracking to find phase change for DIAMOND_A4#1
 Global test at  7.95833E+02 .... OK
 Global check of adding phase at  7.95274E+02
 Calculated   123 equilibria

 Phase Region from    795.274     for:
     LIQUID
```

```
    DIAMOND_A4
    FCC_A1
Global check of removing phase at  7.94976E+02
Calculated     3 equilibria

Phase Region from    794.976     for:
    DIAMOND_A4
    FCC_A1
Calculated     4 equilibria
*** Buffer saved on file: C:\Users\vagrant\AppData\Local\Temp\SCHEIL_26112.POLY3
 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

An EXP file C:\Users\vagrant\AppData\Local\Temp\SCHEIL_EQ_26112.EXP
has been created to store the equilibrium solidification results.
 CALCULATING SCHEIL SOLIDFICATION
FCC_A1#1 set as the primary phase
    T(C)      fraction solid
  641.6828       0.000000
PHASE REGION:LIQUID + FCC_A1
    T(C)      fraction solid
  641.5871      0.3328777E-03
  640.5871      0.5641583E-01
  639.5871      0.1067483
  638.5871      0.1521540
  637.5871      0.1933076
  636.5871      0.2307671
  635.5871      0.2649977
  634.5871      0.2963905
  633.5871      0.3252761
  632.5871      0.3519365
  631.5871      0.3766131
  630.5871      0.3995141
  629.5871      0.4208197
  628.5871      0.4406870
  627.5871      0.4592532
  626.5871      0.4766387
  625.5871      0.4929499
  624.5871      0.5082806
  623.5871      0.5227146
  622.5871      0.5363261
  621.5871      0.5491816
  620.5871      0.5613408
  619.5871      0.5728573
  618.5871      0.5837794
  617.5871      0.5941507
  616.5871      0.6040109
  615.5871      0.6133957
  614.5871      0.6223380
  613.5871      0.6308674
  612.5871      0.6390113
  611.5871      0.6467945
  610.5871      0.6542400
  609.5871      0.6613687
  608.5871      0.6681999
  607.5871      0.6747514
  606.5871      0.6810398
  605.5871      0.6870803
  604.5871      0.6928868
  603.5871      0.6984725
  602.5871      0.7038495
  601.5871      0.7090290
  600.5871      0.7140216
  599.5871      0.7188370
  598.5871      0.7234843
  597.5871      0.7279721
  596.5871      0.7323083
  595.5871      0.7365004
  594.5871      0.7405553
  593.5871      0.7444796
  592.5871      0.7482795
  591.5871      0.7519607
  590.5871      0.7555287
  589.5871      0.7589885
  588.5871      0.7623451
  587.5871      0.7656029
  586.5871      0.7687662
  585.5871      0.7718391
  584.5871      0.7748253
  583.5871      0.7777286
  582.5871      0.7805524
  581.5871      0.7832998
  580.5871      0.7859739
  579.5871      0.7885777
  578.5871      0.7911140
  577.5871      0.7935853
  576.5871      0.7959941
  575.5871      0.7983429
  574.5871      0.8006339
  573.5871      0.8028691
  572.5871      0.8050508
  571.5871      0.8071807
  570.5871      0.8092609
  569.5871      0.8112930
  568.5871      0.8132787
  567.5871      0.8152197
  566.5871      0.8171174
  565.5871      0.8189735
  564.5871      0.8207892
  563.5871      0.8225660
  562.5871      0.8243050
  561.5871      0.8260077
  560.5871      0.8276751
  559.5871      0.8293083
  558.5871      0.8309086
  557.5871      0.8324768
  556.5871      0.8340141
  555.5871      0.8355213
  554.5871      0.8369994
  553.5871      0.8384494
  552.5871      0.8398719
```

```
  551.5871      0.8412680
  550.5871      0.8426383
  549.5871      0.8439836
  548.5871      0.8453046
  547.5871      0.8466021
  546.5871      0.8478767
  545.5871      0.8491291
  544.5871      0.8503600
  543.5871      0.8515698
  542.5871      0.8527593
  541.5871      0.8539289
  540.5871      0.8550793
  539.5871      0.8562109
  538.5871      0.8573243
  537.5871      0.8584200
  536.5871      0.8594984
  535.5871      0.8605600
  534.5871      0.8616052
  533.5871      0.8626345
  532.5871      0.8636484
  531.5871      0.8646471
  530.5871      0.8656311
  529.5871      0.8666008
  528.5871      0.8675566
  527.5871      0.8684988
  526.5871      0.8694278
  525.5871      0.8703438
  524.5871      0.8712473
PHASE REGION:LIQUID + AL2CU_C16 + FCC_A1
    T(C)      fraction solid
  524.1090      0.8717782
  523.1090      0.8774473
  522.1090      0.8826267
  521.1090      0.8873751
  520.1090      0.8917425
  519.1090      0.8957715
  518.1090      0.8994989
  517.1090      0.9029561
  516.1090      0.9061709
  515.1090      0.9091670
  514.1090      0.9119655
  513.1090      0.9145848
  512.1090      0.9170413
  511.1090      0.9193492
  510.1090      0.9215214
  509.1090      0.9235693
  508.1090      0.9255031
  507.1090      0.9273319
  506.1090      0.9290639
  505.1090      0.9307065
  504.1090      0.9322664
  503.1090      0.9337495
  502.1090      0.9351615
  501.1090      0.9365072
  500.1090      0.9377911
  499.1090      0.9390175
  498.1090      0.9401902
  498.0771      0.9402266
PHASE REGION:AL2CU_C16 + C15_LAVES + FCC_A1
    T(C)      fraction solid
  498.0453       1.000000
```

2020.05.11.16.41.36
MALDEMO: AL, CU, SI
T=914.833, X(CU)=2.1E-2, X(SI)=1E-2, P=1E5, N=1




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

       The following axis variables are available

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

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

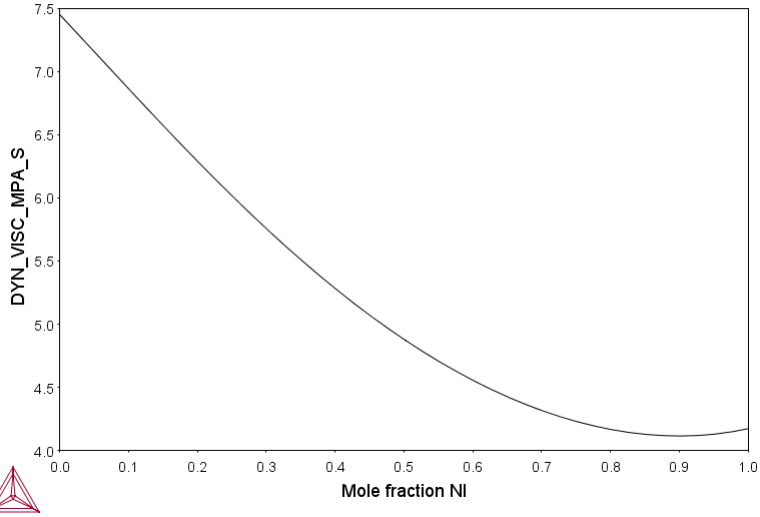
.....

POST:
POST: BACK
SCHEIL: SET-INTER
--OK---
SCHEIL:

tcex55-tcex55.tcm

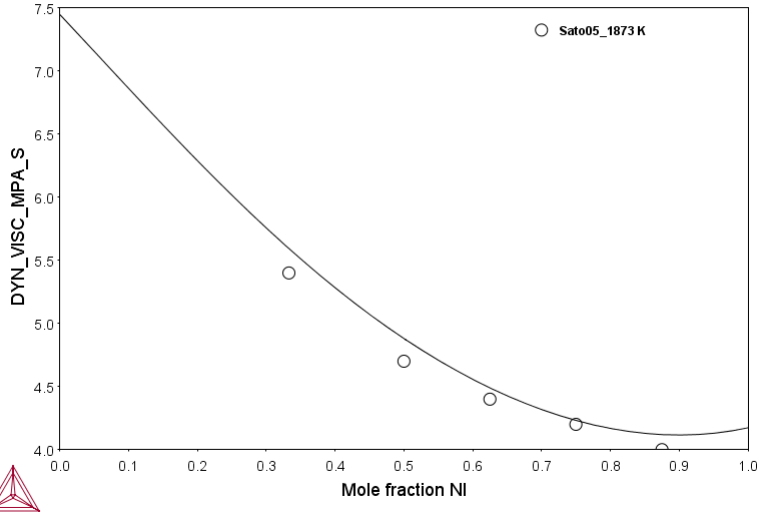
```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

 Copyright Foundation for Computational Thermodynamics,
 Stockholm, Sweden

 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex55\tcex55.tcm.test"
SYS:
SYS: @@ Plotting viscosity of Cr-Ni at 1873 K
SYS:
SYS: set-echo
SYS:
SYS: go da
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw FEDEMO
 Current database: Iron Demo Database v3.0

 VA                      /-  DEFINED
TDB_FEDEMO: def-system ni cr
 NI                      CR  DEFINED
TDB_FEDEMO: reject-phase *
 LIQUID:L                BCC_A2                  LAVES_PHASE_C14
 CBCC_A12                CHI_A12                 CUB_A13
 FCC_A1                  HCP_A3                  SIGMA
   REJECTED
TDB_FEDEMO: restore-phase liquid
 LIQUID:L  RESTORED
TDB_FEDEMO: get
16:43:15,627 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A.T. Dinsdale, SGTE Data for Pure Elements, CALPHAD, 15 (1991) 317-425'
  'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
  'M. Ghasemi, Thermo-Calc Software AB, Sweden, 2019'
  'J. Brillo and I. Egry, Int. J. Thermophysics, 24, 1155-1170'
  'M. J. Assael, High Temp. High Press., 41 (2012); Sb, Pb, Bi, Ni, Ag'
  'B.J. Lee, CALPHAD, 16 (1992) 121-149; C-Cr-Fe-Ni'
 -OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly

 POLY version  3.32
POLY: s-c t=1873 n=1 p=1e5 x(ni)=.2
POLY: c-e
 Using global minimization procedure
Calculated           209 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: s-a-v 1 x(ni) 0 1 ,,
POLY: step sep

 Phase Region from   0.502463     for:
     LIQUID

 Phase Region from   0.502463     for:
     LIQUID
 *** Buffer saved on file *** C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: ent-sym fun Dyn_visc_mPa_s=DVIS(liquid)*1000;
POST: s-d-a y Dyn_visc_mPa_s
POST: s-d-a x m-f ni
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

2020.05.11.16.43.19
FEDEMO: CR, NI
T=1873, N=1, P=1E5



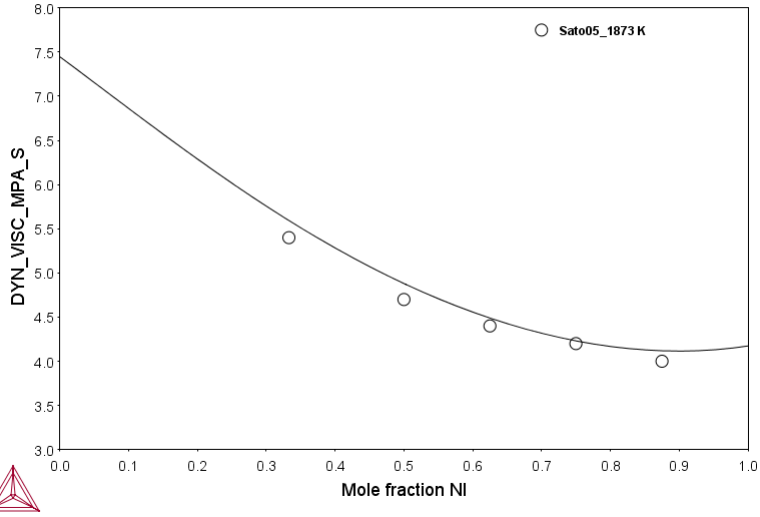

```
POST:
POST: ap-ex y Cr-Ni_1873K.exp 1:1
POST: pl
```

2020.05.11.16.43.19
FEDEMO: CR, NI
T=1873, N=1, P=1E5



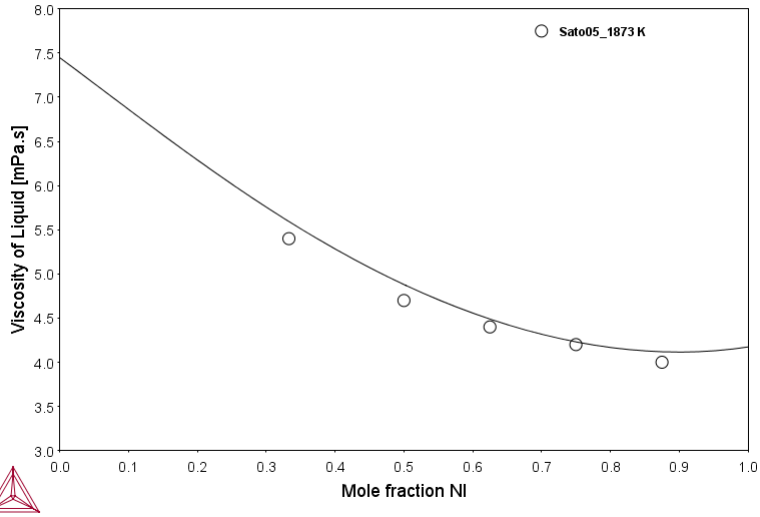

```
POST: s-s-s y n 3 8
POST: pl
```

2020.05.11.16.43.41
FEDEMO: CR, NI
T=1873, N=1, P=1E5




```
POST:
POST:
POST: set-axis-text y N Viscosity of Liquid [mPa.s]
POST: pl
```

2020.05.11.16.44.03
FEDEMO: CR, NI
T=1873, N=1, P=1E5




```
POST:
POST: set-inter
POST:
```

tcex56-tcex56.tcm

```
SYS:About

 Thermo-Calc / DICTRA is software package for calculation of phase diagrams,
 simulation of phase transformation kinetics and much more.

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 Software  (build 22110) running on WinNT 64-bit wordlength
 Compiler: Intel(R) Visual Fortran Compiler Version 16.0.4.246 Build 20160811
 License library version: 8.5.1.0017
 Linked: Mon May 11 13:11:40 2020


SYS:SYS:MACRO "c:\jenkins\workspace\thermocalc_generate_console_examples\examples\tcex56\tcex56.tcm.test"
SYS: @@ Plotting Surface Tension of Cu-Zr at 1373 K
SYS:
SYS: set-echo
SYS:
SYS: go data
 THERMODYNAMIC DATABASE module
 Database folder: C:\jenkins\workspace\thermocalc_generate_console_examples\data
 Current database: Steels/Fe-Alloys  v10.1

 VA                      /-  DEFINED
 DICTRA_FCC_A1  REJECTED
TDB_TCFE10: sw aldemo
 Current database: Aluminum Demo Database v4.0

 VA                      /-  DEFINED
TDB_ALDEMO:
TDB_ALDEMO: de-system cu zr
 CU                      ZR  DEFINED
TDB_ALDEMO: rej-phase *
 LIQUID:L                AL2CU_C16               ALCU_EPS
 ALCU_ETA                ALZR2_B82               BCC_A2
 BCC_B2                  C14_LAVES               C15_LAVES
 C36_LAVES               FCC_A1                  HCP_A3
   REJECTED
TDB_ALDEMO: res-phase liquid
 LIQUID:L  RESTORED
TDB_ALDEMO: get
16:45:42,602 INFO  *** Invoking Gibbs Energy System v6 ***
 REINITIATING GES .....
 ELEMENTS .....
 SPECIES ......
 PHASES .......
 PARAMETERS ...
 FUNCTIONS ....

 List of references for assessed data

  'A. Dinsdale, Calphad,15 317-425 (1991)'
  'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
      Molar volumes'
  'H-L Chen, in TCAL7.0, Evaluation and modeling of electrical resistivity
      thermal conductivity'
  'M J Assael, J Phys Chem Ref Data 39 (2010) 033105; Cu, Sn'
  'M Ghasemi, Thermo-Calc Software AB (2020)'
  'A. Dinsdale, pure elements, volume, private communication, 2004'
  'T Ishikawa, Meas Sci Technol 23 (2012) 025305; Ti, Ni, Zr, Nb, Ru, Rh, Hf,
       Ir, Pt, Tb'
  'I. Ansara (Editor), COST 507, (1998)'
  'M Ghasemi, Thermo-Calc Software AB (2019)'
 -OK-
TDB_ALDEMO:
TDB_ALDEMO: go poly

 POLY version  3.32
POLY: s-c t=1373 n=1 p=1e5 x(zr)=.2
POLY: c-e
 Using global minimization procedure
Calculated           209 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:

POLY: set-axis-var 1 x(zr) 0 1 ,,
POLY: step sep

 Phase Region from   0.502463     for:
     LIQUID

 Phase Region from   0.502463     for:
     LIQUID
 *** Buffer saved on file *** C:\Users\vagrant\AppData\Local\Temp\RESULT_002.POLY3
POLY:
POLY: post
  POLY-3 POSTPROCESSOR VERSION 3.2
POST: set-diagram-axis y surf(liq)
POST: set-diagram-axis x m-f zr
POST:
POST: ap-exp y  Cu-Zr_ALDEMO.exp 1:1
POST:
POST:
POST: set-axis
  Ambiguous command use HELP
POST: set-axis-te
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT  (Y OR N) /N/: N
AXIS TEXT : Surface Tension [J/m2]
POST: pl
```
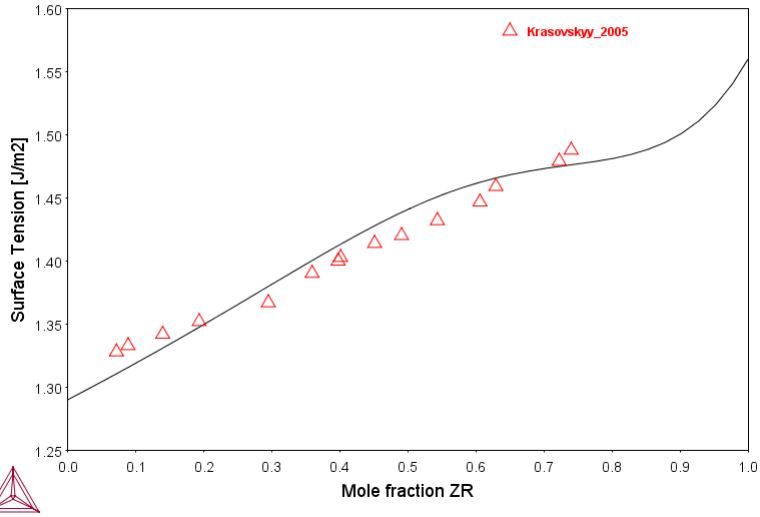
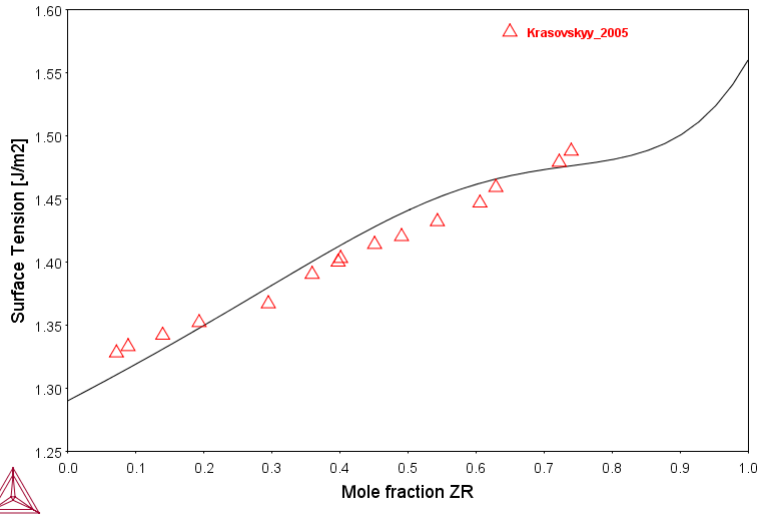

2020.05.11.16.45.46
ALDEMO: CU, ZR
T=1373, N=1, P=1E5




```
POST:
POST:
POST: SET_EXP_FILE_FORMAT 5
POST: MAKE c:/jenkins/workspace/thermocalc_generate_console_examples/unite/distribution\macroResult.exp Y
POST: SET_EXP_FILE_FORMAT 10
POST:
POST: plot
```

2020.05.11.16.46.08
ALDEMO: CU, ZR
T=1373, N=1, P=1E5




```
POST:
POST: set-inter
POST:
```

This page was generated 2020-05-11 16:47